DESCRIPTION

HUMAN-DERIVED PROTEINS FORMING DOMAIN AND USE THEREOF

Technical Field

The present invention relates to a human-derived protein forming a domain, a polynucleotide comprising the same, an antibody against the protein, and a method for screening an active compound using them.

Background Art

Recently, genome nucleotide sequences of various model organisms, as represented by the human genome project, have been decoded one after another. "Structural genomics" is rapidly recognized as a new research area, and large-scale projects are progressing around the world. With respect to a large number of genes extracted from a mass of information about genomic sequences, structural genomics aims at systematic clarification of three-dimensional structure of a protein encoded by each gene and defining structure-function relationship.

In structural genomics, the number of proteins to be analyzed is considered to be 100,000 kinds, and it is not realistic to have a goal to determine the three-dimensional structures of all the proteins at present technical level.

Thus, it is first necessary to narrow down the number of target proteins to a reasonable number and select "representative structures". As a comprehensive three-dimensional structure analysis, projects having selected analysis targets from various viewpoints are initiated: for example, a) specifying relatively small sets of proteins as targets; b) specifying the kind of organisms having a small genome size such as hyperthermophilic archaebacterium, extreme thermophile, and mycoplasma; c) specifying life phenomena, such as signal transduction proteins as

disease-associated gene products, and proteins involved in signal transmission or gene expression.

In the flow of this research, as the first step, it is one goal to determine one or more representative three-dimensional structure regarding all the families, the number of which is predicted to be about 10, 000 (classified as family when amino acid sequences have about 30 to 35% homology). When one representative three-dimensional structure (basic structure) is obtained, structures of other proteins belonging to the same family can be analogized by modeling based on homology.

In this project, attention is drawn to the type of three-dimensional structure or the topology (basic structure: fold) of a functional domain, and research to clarify the correlation with a function for a basic structural unit of protein receives attention.

A protein having a plurality of domains is formed by combining functional domains like a module, and thus it is frequent that one domain appears in various proteins with the combination of different domains. Further, even if homology is not detected on a primary sequence, it is not unusual that proteins have the same basic structure. Therefore, the number of types of basic structures must be much smaller than the number of protein families, and it is expected that individual basic structures are associated with molecular functions. The number of the basic structures is predicted to be about 10,000 to 20,000, and if the analysis targets are within this number order it is sufficiently possible to determine the three-dimensional structures of all the target proteins.

Thus obtained information regarding the three-dimensional structure and functions of protein provides new findings for elucidation of vital functions, and makes a dramatic progress in developing drugs etc. (e.g. development by rational drug design or virtual screening). Therefore, such information is very useful in the industry.

Disclosure of the Invention

However, the fact is that three-dimensional structure analysis of protein requires a lot of time, labor and cost. In structural genomic research aiming at comprehensive and systematic structure analysis, it is an important challenge to attain high throughput structure analysis.

For the analysis of a three-dimensional structure of protein, NMR method and X-ray crystallography are mainly used.

To analyze a three-dimensional structure of protein using NMR, it is preferable that a sample has a molecular weight of about 20,000 or less (about 200 or less amino acid residues). In the case of analysis of the three-dimensional structure by X-ray analysis, the properties of proteins are limited due to preparation of crystals.

When a protein is randomly cleaved to obtain a protein suitable for structure analysis and a cleavage site exists in an amino acid sequence having a β -sheet or α -helix structure, many proteins modify their physiologically significant structures, become a string-like shape not taking a structure, or aggregate. In this way, it is meaningless to analyze a three-dimensional structure of protein not having an original in vivo structure. Therefore, it is desirable to obtain a protein forming a significant domain for three dimensional analysis.

To express a protein having a domain suitable for structural analysis (hereinafter referred to as "a protein forming a domain"), information regarding the position of domain boundary is necessary. In general, such domain boundary is predicted using amino acid sequence homology or the like as a clue. Even if protein expression is conducted based on the amino acid sequence of the thus predicted domain region, there is very low probability that a protein forming a domain actually having a structure (folding) is obtained and thus domain expression is one of bottlenecks in structure analysis.

A protein forming a CAP-Gly-like domain of the present invention has not been obtained so far, and the structure information thereof is unknown. Thus, these cannot be used for the drug discovery.

Disclosure of the Invention

In view of such circumstances, the present invention has been accomplished, and the present invention provides a protein described below, a production method thereof, a polynucleotide coding therefor, an antibody against the protein, and a screening method using them.

- (1) A protein consisting of an amino acid sequence represented by SEQ ID NO:1, or a salt thereof.
- (2) A protein consisting of an amino acid sequence represented by any one of SEO ID NOS:3, 5, and 7, or a salt thereof.
- (3) A protein having an amino acid sequence derived from an amino acid sequence represented by SEQ ID NO:5 by deletion of 0 to 10 amino acid residues from the N-terminal and deletion of 0 to 5 amino acid residues from the C-terminal and having 92 to 106 amino acid residues, or a salt thereof.
- (4) A protein consisting of an amino acid sequence derived from an amino acid sequence of a proteins according to any one of the above (1), (2), and (3) and having deletion, substitution or addition of one to several amino acids and having a function substantially identical with that of the protein according to the above (1), (2), or (3), or a salt thereof.
- (5) A polynucleotide comprising a polynucleotide encoding an amino acid sequence of any one of proteins according to the above (1) to (4).
- (6) The polynucleotide according to the above (5), containing a nucleotide sequence represented by any one of SEQ ID NOS:2, 4, 6, and8

- (7) A recombinant vector containing a polynucleotide according to the above (5) or (6).
- (8) A transformant which is transformed with a polynucleotide according to the above (5) or (6).
- (9) An antibody against a protein according to any one of the above (1) to (4).
- (10) A method for producing a protein or a salt thereof according to any one of the above (1) to (4), comprising the steps of culturing the transformant of the above (8) and producing the protein.
- (11) A method for producing a protein or a salt thereof according to any one of the above (1) to (4), characterized by using a cell-free protein synthesis system.
- (12) A method for screening a substance interacting with a protein or a salt thereof according to any one of the above (1) to (4) and/or a naturally existing protein or a salt thereof containing an amino acid sequence of a protein according to any one of the above (1) to (4), comprising the steps of bringing a candidate substance into contact with the protein of any one of the above (1) to (4); and confirming whether the candidate substance interacts with the protein.
- (13) A method for assaying a protein or a salt thereof according to any one of the above (1) to (4) using an antibody of the above (9).
- (14) A method for screening a substance interacting with a protein or a salt thereof according to any one of the above (1) to (4) using an assay method of the above (13).
- (15) A method for specifying a gene associated with a protein according to any one of the above (1) to (4), comprising the steps of expressing the protein according to any one of the above (1) to (4) in a cell; and examining an expression status of the gene in the cell.
- (16) A method for screening a substance interacting with a protein or a salt thereof according to any one of the above (1) to (4) and/or a naturally existing protein or a salt thereof containing an amino acid sequence of a protein according to any one of

the above (1) to (4), comprising the steps of determining an active site of the protein using information concerning three-dimensional structure of the protein according to any one of the above (1) to (4); and specifying a compound interacting with the active site on a computer.

- (17) The screening method according to the above (16), wherein the information concerning three-dimensional structure of the protein is three-dimensional structure information of a protein consisting of amino acid residues from amino acid 8 to amino acid 98 among three-dimensional structure information described in any of three-dimensional structure coordinate tables 1 to 20.
- (18) The screening method according to the above (17), wherein, among three-dimensional structure information described in three-dimensional structure coordinate table 1, a part of information corresponding to amino acid residues (Val26, Lys27, Glu47, Arg67, Lys83 and Ser86) is used.
- (19) A method for screening a substance interacting with a protein or a salt thereof according to any one of the above (1) to (4) and/or a naturally existing protein or a salt thereof containing an amino acid sequence of a protein according to any one of the above (1) to (4), wherein a compound interacting with a specified active site is prepared as a candidate compound by a screening method according to any one of the above (16) to (18), the method comprising the steps of bringing the candidate substance into contact with a protein according to any one of the above (1) to (4); and confirming whether the candidate substance has interaction with the protein.
- (20) A method for presuming a three-dimensional structure of a protein with an unknown structure, wherein homology modeling is conducted on the protein with an unknown structure comprising an amino acid sequence having 30% or more homology with an amino acid sequence of a protein according to any one of the above (1) to (4), by using information concerning three-dimensional structure information of a protein having amino acid residues from amino acid 8 to amino acid

98 among three-dimensional structures of a protein described in any of three-dimensional structure coordinate tables 1 to 20.

Brief Description of the Drawings

Fig. 1 shows SDS gel electrophoregrams of Examples 1 to 4. Fig. 1A shows an SDS gel electrophoregram of Example 1, Fig. 1B shows an SDS gel electrophoregram of Example 2, Fig. 1C shows an SDS gel electrophoregram of Example 3, and Fig. 1D shows an SDS gel electrophoregram of Example 4;

Fig. 2 shows SDS gel electrophoregrams of respective Comparative Examples. Fig. 2A shows an SDS gel electrophoregram of Comparative Example 1, Fig. 2B shows an SDS gel electrophoregram of Comparative Example 2, and Fig. 2C shows an SDS gel electrophoregram of Comparative Example 3;

Fig. 3 shows one-dimensional nuclear magnetic resonance spectrum and $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum of the protein represented by SEQ ID NO:1. Fig. 3A shows a one-dimensional nuclear magnetic resonance spectrum and Fig. 3B shows a $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum;

Fig. 4 shows one-dimensional nuclear magnetic resonance spectrum and $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum of the protein represented by SEQ ID NO:3. Fig. 4A shows a one-dimensional nuclear magnetic resonance spectrum and Fig. 4B shows a $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum;

Fig. 5 shows one-dimensional nuclear magnetic resonance spectrum and $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum of the protein represented by SEQ ID NO:5. Fig. 5A shows a one-dimensional nuclear magnetic resonance spectrum and Fig. 5B shows a $^{1}\text{H-}^{15}\text{N}$ HSQC spectrum;

Fig. 6 shows one-dimensional nuclear magnetic resonance spectrum and ¹H-¹⁵N HSQC spectrum of the protein represented by SEQ ID NO:7. Fig. 6A shows a one-dimensional nuclear magnetic resonance spectrum and Fig. 6B shows a ¹H-¹⁵N HSQC spectrum;

Fig. 7 is a graph showing measurement results of viable cell count using 293 cells and HeLa cells; and

Fig. 8 is a photograph, instead of a figure, showing a detected image of western blotting in Example 9. Lane 1 is a lane of only a supernatant of HeLa cell extract (control), lane 2 is a lane of a product wherein IKK-gamma (1-419) and a FLAG sequence were expressed in a HeLa cell (control), and lane 3 is a lane of a product wherein IKK-gamma (1-419) and addition of a FLAG sequence to a CAP-Gly-like domain protein (464-554) were expressed in a HeLa cell.

Best Mode for Carrying Out the Invention (Protein of the present invention)

A protein of the present invention is a protein forming a domain with a three-dimensional structure. More particularly, the present invention relates to a CAP-Gly-like domain protein represented by any one of SEQ ID NOS:1, 3, 5, and 7, or a protein having an amino acid sequence derived from an amino acid sequence represented by SEQ ID NO:5 by deletion of 0 to 10 amino acid residues from the N-terminal and deletion of 0 to 5 amino acid residues from the C-terminal and having 92 to 106 amino acid residues (that is, a protein wherein 0 to 10 amino acid residues and 0 to 5 amino acid residues are added to N-terminal and C-terminal of SEQ ID NO:1, respectively).

Hereinafter, the protein of the present invention will be described in terms of functions and the like.

CAP-Gly is an abbreviation of

cytoskeletal-associated-protein-glycine-conserved domain, and constitutes a protein having a role for combining an intracellular minute organ or a chromosome with an intracellular microtubule. A CAP-Gly domain includes highly preservative region

abundant in glycin comprising about 42 residues [Riehemann K., Sorg C. Sequence homologies between four cytoskeleton-associated proteins. Trends Biochem. Sci. 18: 82-83(1993)]. As a protein containing this domain, there are known: restin, a protein of 160 kDa pertaining to an intermediate filament connecting an intracellular endoplasmic reticurum to a microtubule (also called as cytoplasmic linker protein 170 or CLIP-170); dynactin of vertebra [dynein associated polypeptide of 150 kDa (DAP)]; Drosophila glued complex which is a main component of activator I; yeast protein BIK1 which is considered necessary for the formation and stabilization of microtubules at mitosis and for spindle fusion at pairing; yeast protein NIP100 (NIP80); human protein CKAP1/TFCB; alp11 of Schizosaccharomyces pombe protein; and F53F4.3 which is presumed a protein of C. elegans. Further, with respect to the relation between a CAP-Gly-like domain protein and diseases, Examples have shown that CAP-Gly-like domain has cell proliferation inhibition effect and that CAP-Gly-like domain binds to IKK-gamma. It is accordingly predicted that the CAP-Gly-like domain is a causative gene of protein exhibited proliferation inhibition effect in HeLa cells (uterine cervix cancer cells) and 293 cells. In Example 9, the protein exhibited an ability to bind to IKK-gamma. Here, IKK-gamma is a factor which binds to a transcription factor NF-kB to inhibit transcription enhancing function of NF-kB. Further, NF-kB is formed as a heterocomplex from p50 and p65 derived from oncogenes of the Rel family. The CAP-Gly-like domain binds to IKK-gamma and exhibits proliferation inhibition activity, and it can be thus considered that its binding to IKK-gamma inhibits transcription enhancement of NF-kB. In this way, inhibition of cell proliferation is controlled by the CAP-Gly-like domain, and therefore the protein of the present invention has a function as a cancer suppressor gene product. It is a well-known fact that when a mutation in a cancer suppressor gene and lowered

proliferation inhibition activity lead to the onset of cancer (Yoichi Taya et al., Bio Science Term Library, Cancer Gene-Cancer suppressor gene, pp. 113-115, Yodosha, 2000). Retinoblastoma gene is well known, which causes retinoblastoma (Weinberg RA. The retinoblastoma protein and cell cycle control. Cell 81, 323-330 1995). Particularly, a gene (KIAA0849) used of the present invention is known as a causative gene of human Turban tumor syndrome (Nature Genet. 25, 160-165 2000). Still, it is unknown which domain of the protein expressed by KIAA0849 is a cause to the disease. However, in consideration of the cancer suppressing genetic function of the protein of the present invention, as exemplified by the present invention, CAP-Gly-like domain protein is predicted to be a cause of the disease. As application of the present invention, screening of drugs for Turban syndrome and optimizing a drug using three-dimensional structure information are assumed. It can be effectively used for the prevention and treatment of various cancer-related diseases.

Further, the present invention provides: a protein or a salt thereof consisting of an amino acid sequence represented by any one of SEQ ID NOS: 1, 3, 5, and 7, or an amino acid sequence derived from the amino acid sequence represented by SEQ ID NO:5 by deletion of 0 to 10 amino acid residues from the N-terminal and deletion of 0 to 5 amino acid residues from the C-terminal, which further comprises by deletion, substitution or addition of one to several (1 to 9, preferably 1 to 5, more preferably 1 to 2) amino acids and which has a function substantially identical to that of the protein consisting of an amino acid sequence derived from the amino acid sequence represented by SEQ ID NO:5 by deletion of 0 to 10 amino acid residues from the N-terminal and deletion of 0 to 5 amino acid residues from the C-terminal.

It should be noted that the term "having a cell proliferation inhibition function substantially identical to that of the protein of the present invention" means to have the same cell proliferation inhibition function as the protein of the present invention

has. Here, such molecular functions include functions and activities of the CAP-Gly-like domain protein in addition to connectivity with IKK-gamma.

IKK-gamma is an abbreviation of inhibitor-kappaB, and binds to NF(Nuclear Factor)-kB. NF-kB is a transcription factor that binds to an intron enhancer of immunoglobulin kL chain gene, and is a heterodimer composed of two kinds of subunits, p50 and p65. Here, both p50 and p65 exhibit homology with oncogene Rel and belong to the Rel family. As its function, NF-kB was initially considered to be specific to a B cell and to control the expression of a cell specific gene that is expressed as the B cell differentiates. Thereafter, the same effect was also observed to a non-B cell. Further, NF-kB binds to transcription control regions of various genes in addition to an immunoglobulin gene, and activates the transcription of these genes. In a non-B cell, an inactive NF-kB binds to IKK-gamma thereby to form a complex. IKK-gamma is inactivated by phosphorylation induced by extracellular stimulation. As a result, NF-kB is dissociated and transferred into each nucleus thereby to be activated, so that it functions as a transcription factor. As subunits of IKK-gamma, IKK-α, IKK-β, and bcl-3 are known.

(Sequence of protein)

The sequencing of the protein of the present invention is conducted as follows: i) presuming a domain region having a function of interest based on known protein sequence information; ii) preparing domain candidate sequence patterns having a basic pattern as the amino acid sequence of the thus presumed domain; iii) expressing a protein of each sequence pattern, evaluating structural stability of the obtained protein forming the domain, using a protein having a good result as a domain of interest, and defining each protein according to the amino acid sequence of the domain of interest. In other words, the protein of the present invention is empirically selected so as to have a stable structure when a part (having a function of

interest) of the full length protein is fragmented and expressed as a protein forming a domain. There exist domain candidates in the order of 100 at the stage of domain region prediction, but the number of domain candidates is narrowed down due to various factors and in fact carefully selected in the order of 10 to several tens. Therefore, use of thus selected proteins in three-dimensional structure analysis enables highly accurate and reliable structure analysis.

(Presumption of domain region)

A method for presuming a domain region in the full length protein is not particularly limited, and any of the following methods can be used: information science methods such as bioinformatics or computational science methods (see the specification of Japanese Patent Application No. 2001-309434), combination of deleted DNA library and GFP (see the specification of Japanese Patent Laid Open No. 2002-262873), and experimental methods such as limited breakdown (proteolysis) by protease. By using more accurate methods, the efficiency to select a domain of interest from domain candidates is improved. (Production of domain candidate sequence pattern)

The above domain candidate sequence patterns are produced by extending or shortening the position of domain boundary to the N- or C- terminals on the basis of the above presumed domain region.

For example, prepared is a domain candidate sequence pattern having about several tens of kinds of new boundaries as the N-terminal, which are provided by extending several to tens of residues to the N-terminal or shortening several to tens of residues the C-terminal, from the position of the amino acid residue in the domain boundary at the N-terminal of the presumed domain region. Similarly, produced is a domain candidate sequence pattern having several kinds of domain boundaries as the C-terminal, which are selected in the domain boundary at the C-terminal of the presumed domain region.

(Extending and shortening of domain boundary)

As a method for extending or shortening a domain boundary of the above presumed domain region, employed is, for example, a method for synthesizing individual PCR primers capable of producing cDNAs corresponding to the above domain candidate sequence patterns and performing the creation by PCR. In particular, 2-step PCR method described in Japanese Patent Laid Open No.2003-9880 is suitable.

(Extraction of target domain from domain candidate sequence pattern)

In order to select a target domain having actually stable three-dimensional structure from the above domain candidate sequence patterns, protein synthesis is performed using cDNA of domain candidate sequence pattern produced as mentioned above.

An expression system for the domain candidate sequence pattern is not particularly limited, and any of conventionally known expression systems are usable.

Next, it is determined whether the obtained protein actually has a stable three-dimensional structure, and when a protein confirmed to have such three-dimensional structure is used as a protein in the present invention.

Examples of indicators for the stability of three-dimensional structure of protein include: biochemical indicators such as an indicator whether a synthesized domain protein is detected as soluble protein by SDS gel electrophoresis, etc. and also detected as uniform band corresponding to a proper molecular weight; and spectroscopic methods having as an indicator fluorescence strength of GFP fused at the C-terminal side, NMR spectrum, and CD spectrum.

The conventional process of determining a protein sequence has problems in that, for example, (1) a protein forming a target domain is not expressed in the above protein synthesis, or (2) though the protein is expressed, it causes aggregation or has

low solubility, etc. The present inventors have overcome these problems and completed the present invention.

(Confirmation of having stable three-dimensional structure)

Regarding the above NMR spectrum, the determination for folding of a protein forming a domain is shown below.

When a protein forming a domain is not folded in 1D spectrum, signals derived from methyl group proton such as Val, Leu, and Ile are observed around 0.8 ppm. However, when a protein is folded, the environment of methyl group proton is changed and signals are shifted to higher magnetic field side (around 0.7 ppm to -0.5 ppm).

The determination in ¹H-¹⁵NHSQC can be made by visual evaluation of the cross peak convergence degree and the uniformity of signal strength. In other words, when cross peaks are densely gathered, the status is considered not forming a three-dimensional structure. Conversely, when dispersed, the status is considered forming a stable three-dimensional structure. In this way, the stability of three-dimensional structure is evaluated.

(Vector)

A (recombinant) vector of the present invention can be obtained by ligating (inserting) a gene of the present invention into a proper vector. The vector for inserting the gene of the present invention thereinto is not particularly limited as long as it can be replicated in a host cell. Examples thereof include plasmid DNAs and phage DNAs.

Specific examples of the plasmid DNAs include *E. coli*-derived plasmids (e.g. pRSET, pBR322, pBR325, pUC118, pUC119, pUC18, and pUC19), *Bacillus subtilis*-derived plasmids (e.g. pUB110 and pTP5), yeast-derived plasmids (e.g. YEp13, YEp24, and YCp50). Specific examples of the phage DNAs include λ phage (Charon4A, Charon21A, EMBL3, EMBL4, λ gt10, λ gt11, and λ ZAP).

Further, animal viruses such as retrovirus and vaccinia virus and insect virus vectors such as baculovirus can be used.

To insert a gene of the present invention into a vector, a method is employed, which comprises first cleaving a purified DNA with a proper restriction enzyme and inserting the gene to a restriction enzyme site of a proper vector DNA or a multicloning site to ligate to the vector.

It is necessary for the gene of the present invention to be incorporated into a vector so that the gene exhibits its function. Hence, in addition to a promoter and the gene of the present invention, an enhancer or the like including a cis-element, a splicing signal, a poly A addition signal, a selective marker, and a ribosome junction sequence (SD sequence) can be ligated into the vector of the present invention, if desired. Further, examples of the selective makers include a dihydrofolate reductase gene, an ampicillin resistance gene, and a neomycin resistance gene. (Transformant)

A transformant of the present invention can be obtained by introducing a polynucleotide of the present invention into a host so that a gene of interest can be expressed therein. Due to easiness and good efficiency, vectors are used for transformation in many cases. Herein, a host is not particularly limited, as long as it can express DNA of the present invention. Examples thereof include bacterium belonging to genus *Escherichia* such as *Escherichia coli*, genus *Bacillus* such as *Bacillus subtilis*, genus *Pseudomonas* such as *Pseudomonas putida*, genus *Rhizobium* such as *Rhizobium meliloti*. Further, yeasts such as *Saccharomyces cerevisiae* and *Schizosaccharomyces pombe*, and animal cells such as COS cells and CHO cells can be used. Or insect cells such as Sf9 and Sf21 can be used.

When a bacteria such as *E. coli* is a host, it is preferable that the recombinant vector of the present invention comprises a promoter, a ribosome junction sequence, a gene of the present invention, and a transcription termination sequence while

autonomously replicable in the bacteria. In addition, a gene to control the promoter may be contained.

Examples of *E. coli* include *E. coli* K12 and DH1 and examples of *Bacillus subtilis* include *Bacillus subtilis*. As a promoter, anyone can be used as long as it can be expressed in a host such as E. coli. Promoters derived from *E. coli* or phages such as trp promoter, lac promoter, P_L promoter, and P_R promoter can be used. Artificially designed and modified promoters such as tac promoter can be used. A method for introducing a recombinant vector into a bacteria is not particularly limited, as long as it is a method for introducing a DNA into bacteria. There are, for example, a method using calcium ion (Cohen, S.N. et al. (1972) Proc. Natl. Acad. Sci., USA 69, 2110-2114) and electroporation method.

When yeast is a host, *Saccharomyces cerevisiae*, *Schizosaccharomyces pombe*, and *Pichia pastor* is, for example, are used. In this case, a promoter is not particularly limited as long as it can be expressed in yeast. Examples thereof include gal1 promoter, gal10 promoter, a heat shock protein promoter, MFα1 promoter, PHO5 promoter, PGK promoter, GAP promoter, ADH promoter, and AOX1 promoter. A method for introducing a recombinant vector into a yeast is not particularly limited as long as the method can introduce a DNA into a yeast. Examples of the methods include electroporation method (Becker, D.M. et al. (1990) Methods. Enzymol., 194,182-187), spheroplast method (Hinnen, A. et al. (1978) Proc. Natl. Acad. Sci., USA 75, 1929-1933), and lithium acetate method (Itoh, H. (1983) J. Bacteriol. 153,163-168).

When an animal cell is a host, a monkey cell COS-7, Vero, Chinese hamster ovary cell (CHO cell), a mouse L cell, a rat GH3, and a human FL cell can be used. As a promoter, SRα promoter, SV40 promoter, LTR promoter, and CMV promoter can be used, and further an early gene promoter of human cytomegalovirus may be used. Examples of the methods for introducing a recombinant vector into an animal

cell include electroporation method, calcium phosphate method, and lipofection method.

When an insect cell is a host, an Sf9 cell, an Sf21 cell or the like may be used. As a method for introducing a recombinant vector into an insect cell, calcium phosphate method, lipofection method, and electroporation method may be used, for example.

(Antibody)

Using the protein of the present invention as an antigen, an antibody against the antigen can be prepared.

[Production of a polyclonal antibody against the protein of the present invention]

An animal is immunized using the aforementioned antigen. In the case of a rabbit, a dose per animal of an antigen is 100 to 500 µg using, for example, an adjuvant. As the adjuvant, Freund's complete adjuvant (FCA), Freund's incomplete adjuvant (FIA), aluminum hydroxide adjuvant, etc. are used.

Immunization is carried out by administration to mammalians (e.g. non-human mammalians such as a rat, a mouse, and a rabbit). Administration is conducted intravenously, hypodermically, or intraperitoneally. In addition, immunization interval is not particularly limited, and it may be several-day to several-week interval, preferably 2- to 3-week interval. At such interval, an animal is immunized 1 to 10 times, preferably 2 to 3 times. After 6 to 60 days from final immunization, antibody titer is measured. On a day when the greatest antibody titer is exhibited, blood is collected to obtain antiserum. The antibody titer is measured by ELISA (enzyme-linked immunosorbent assay), RIA (radioimmuno assay), or the like.

When purification of an antibody is needed from antiserum, the purification can be conducted by properly selecting a well-known method such as ammonium

sulfate precipitation method, ion exchange chromatography, gel filtration, and affinity chromatography, or combination thereof.

[Production of a monoclonal antibody against the protein]

An animal is immunized using the aforementioned antigen. If necessary, an adjuvant (commercially available Freund's complete adjuvant, Freund's incomplete adjuvant, etc.) may be mixed in the same manner as above to perform immunization effectively.

Immunization is carried out by administration to mammalians (e.g. a rat, a mouse, and a rabbit). A dose per mouse of an antigen is 50 µg. Administration is conducted mainly intravenously, hypodermically, or intraperitoneally. Further, immunization interval is not particularly limited, and it may be several-day to several-week interval, preferably 2- to 3-week interval at least two to three times. Then, antibody-producing cells are collected after final immunization. As an antibody-producing cell, there are a spleen cell, a lymph node cell, a peripheral blood cell, or the like, but a spleen cell is preferable.

[Cell fusion]

To obtain a hybridoma, cell fusion of an antibody producing cell and a myeloma cell is performed. As a myeloma cell to be fused with an antibody producing cell, an established cell line can be used, which is generally available and derived from an animal such as a mouse. Preferably used is a cell line which has drug selectivity, and has properties whereby it is unable to survive in HAT selective medium (containing hypoxanthine, aminopterin, and thymidine) without the fusion but able to survive only with the fusion with an antibody producing cell. Specific examples of myeloma cells include mouse myeloma cell lines such as P3X63-Ag.8.U1(P3U1), P3/NSI/1-Ag4-1, and Sp2/0-Ag14.

Next, cell fusion of the above myeloma cell with an antibody producing cell is performed. In an animal cell culture medium such as DMEM and RPMI-1640

medium without inclusion of serum, antibody producing cells and myeloma cells are mixed in the ratio of 15:1 to 25:1. Fusion reaction is performed in the presence of a cell fusion accelerator such as polyethylene glycol, or by electric pulse treatment (e.g. electroporation).

[Selection and cloning of hybridoma]

From cells treated by cell fusion, a hybridoma of interest is selected. For example, the treated cells are cultured in a medium containing hypoxanthine, aminopterin and thymidine, and growing cells are obtained as a hybridoma.

Next, screening is performed to determine whether an antibody of interest exists in a culture supernatant of increased hybridoma. The screening of hybridoma may be performed, without particular limitation, in a conventional manner. For example, a part of culture supernatant grown as hybridoma in a well is collected, and screened by ELISA (enzyme-linked immunosorbent assay), RIA (radioimmuno assay) or the like. Cloning of fused cells is performed by limiting dilution method or the like, and finally a hybridoma of a monoclonal antibody producing cell is established.

[Collection of monoclonal antibody]

As a method for collecting monoclonal antibodies from established hybridoma, a conventional cell culture method or the like may be employed. In the cell culture method, the hybridoma is cultured for 3 to 10 days under ordinary culture conditions (e.g. 37°C, 5% CO₂ concentration) in an animal cell culture medium such as RPMI-1640 or MEM media containing 10% bovine fetus serum, and antibodies are collected from resultant culture supernatant.

In the above antibody collection method, antibodies can be purified, if necessary, by properly selecting a well-known method such as ammonium sulfate precipitation method, ion exchange chromatography, affinity chromatography, and gel chromatography, or combination thereof.

(Production of the protein of the present invention)

The protein of the present invention can be obtained by culturing a transformant and collecting the protein from the culture. The term "culture" means, in addition to a culture supernatant, any of a cultured cell, a cultured fungus body, and a matter of crushed cell or fungus body. "A method for culturing a transformant of the present invention" is performed according to a conventional method used for culturing a host.

As a culture medium for culturing the transformant obtained by using microorganisms such as E. coli and yeast as a host, any of natural medium and synthetic medium may be used as long as it contains carbon source, nitrogen source, mineral, etc. which can be utilized as resource by the microorganisms and it effectively cultures the transformant. As the carbon source, used are carbohydrates such as glucose, fructose, sucrose and starch, organic acids such as acetic acid and propionic acid, and alcohols such as ethanol and propanol. As the nitrogen source, used are ammonium salts of inorganic or organic acids such as ammonia, ammonium chloride, ammonium sulfate, ammonium acetate, and ammonium phosphate, or other nitrogen-containing compounds as well as peptone, meat extract, and corn steep liquor. As inorganic matters, monopotassium phosphate, dipotassium phosphate, magnesium phosphate, magnesium sulfate, sodium chloride, ferrous sulfate, manganese sulfate, copper sulfate, and calcium carbonate may be used.

Culture is carried out preferably at 37°C under aerobic conditions such as shaking culture or aerobic culture with stirring for 6 to 24 hours. During the culture period, pH is kept at 7.0 to 7.5. The pH is adjusted preferably by using inorganic or organic acid, alkali solution, etc. During the culture, antibiotics such as ampicillin and tetracycline may be added to the culture medium if necessary.

When a microorganism is cultured which has transformed with an expression vector having used an inducible promoter as a promoter, an inducer may be added to

the medium if necessary. For example, when a microorganism transformed with an expression vector having used Lac promoter is cultured, isopropyl-β-D-thiogalactopyranoside (IPTG), etc. may be added to the medium. When a microorganism transformed with an expression vector having used trp promoter is cultured, indole acrylic acid (IAA) may be added to the medium.

As a medium for culturing a transformant obtained by using an animal cell as a host, RPMI1640 or DMEM media, which are commonly used, or these media having bovine fetus serum added thereto may be used. Culture is carried out at 37°C for 1 to 30 days in the presence of 5% CO₂. During the culture period, antibiotics such as kanamycin, penicillin etc. may be added to the medium.

After the culture, protein is extracted by crushing a fungus body or a cell when the protein is produced in a fungus body or a cell. Further, the protein of the present invention is produced outside a fungus body or a cell, the culture medium is used as it is or the fungus body or cell is removed by centrifugation, etc. Thereafter, the protein of the present invention can be isolated and purified from the above culture medium by using either alone or proper combination of biochemical methods commonly used for isolation and purification of protein, such as ammonium sulfate precipitate, gel chromatography, ion exchange chromatography, affinity chromatography, etc. During or after this purification process, the tag sequence, which was used for purification by protease treatment can be removed. (Method for producing a protein forming a domain using a cell-free protein synthesis system)

Using a cell-free protein synthesis system, the present invention provides a method for producing: a protein comprising an amino acid sequence represented by any one of SEQ ID NOS:1, 3, 5, and 7; and a protein comprising an amino acid sequence derived from the amino acid sequence represented by SEQ ID NO:5 by

deletion of 0 to 10 amino acid residues from the N-terminal and deletion of 0 to 5 amino acid residues from the C-terminal and having 92 to 106 amino acid residues.

A cell-free protein synthesis system is a system in which proteins are synthesized in vitro by using a cell extract. "A cell-free protein synthesis system" includes both a cell-free translation system for synthesizing proteins on ribosome through reading of information of mRNA, and a system including both a cell-free transcription system for synthesizing RNA using DNA as the template and a cell-free translation system. Since a cell-free protein synthesis system can modify a system easily, it has an advantage to easily construct an expression system suitable for a target protein. Further, a cell-free protein synthesis system is described in detail in Japanese Patent Laid Open No. 2000-175695.

[Cell extract]

A crude cell extract may be an extract from eukaryotic or prokaryotic cell in a state of high protein synthesis activity such as bacteria (e.g. *E. coli*), fungi (e.g. budding yeast), wheat germ, rabbit reticulocyte, murine L-cell, Ehrlich ascetic cancer cell, HeLa cell, and CHO cell (Clemens, M.J., Transcription and translation- a practical approach, (1984), pp. 231-270, Henes, B.D. and Higgins, S.J. eds., IRL Press, Oxford).

A crude cell extract preferably contains a component required for protein synthesis such as ribosome and tRNA. For preparation of a crude extract, a method described, for example, in Pratt, J.M. et al., transcription and translation - a practical approach, (1984), pp. 179-209, Henes, B.D. and Higgins, S.J. eds., IRL Press, Oxford, can be used. More specifically, the preparation can be conducted by crushing with a French press (Pratt, mentioned above) or crushing with glass beads. A preferable cell extract is *E. coli* S30 cell extract. S30 extract can be prepared from E. coli BL21 Codon Plus strain in accordance with generally known methods such as a method of Pratt et al. (above mentioned), or S30 extract commercially

available from Promega or Novagen can be used. The cell extract derived mainly from *E. coli*, wheat germ, and rabbit reticulocyte.

[Dialyzer]

A dialyzer which enables shaking or agitating while having internal and external dialysates isolated from each other via a dialysis membrane can be used. Examples of a small-scale reaction apparatus include Dispo Dialyzer (registered trademark) (manufactured by Spectrum) and Slidealyzer (registered trademark) (manufactured by Pierce).

Further, examples of a large-scale reaction apparatus include Spectra/Por (registered trademark) dialysis tube (manufactured by Spectrum).

[Internal dialysate]

In addition to a concentrated cell extract such as E. coli S30, an internal dialysate of a cell-free protein synthesis system, liquid for synthesis of protein, may contain DNA or RNA (mRNA and the like) encoding the target proteins, ATP (adenosine 5'-triphosphate), GTP (guanosine 5'-triphosphate), CTP (cytidine 5'-triphosphate), UTP (uridine 5'-triphosphate), buffer solutions, salts, amino acids, RNase inhibitors, antibacterial agents, RNA polymerase if necessary (in a case where DNA is used as template), and tRNA.

In addition, it can contain ATP regenerating systems such as combinations of phosphoenolpyruvate and pyruvate kinase, or creatine phosphate and creatine kinase, polyethyleneglycol (for example, PEG#8000), 3',5'-cAMP, folic acids, RNase inhibitors, and reducing agents (for example, dithiothreitol). On the other hand, an external dialysate (that is, protein synthesis substrate solution) can use the same composition of the internal dialysate excluding cell extract, RNase inhibitors, DNA or RNA, and RNA polymerase. For example, it may contain buffer solutions, ATP, GTP, CTP, UTP, salts, amino acids, and antibacterial agents. The concentration of added components can be determined arbitrarily.

[Buffer solution]

As the buffer solution, buffer agent such as Hepes-KOH and Tris-OAc can be used, for example. Examples of the salts include acetates (for example, ammonium salts, magnesium salts, and the like) and glutamate salts. Examples of the antibacterial agents include sodium azide and ampicillin. Examples of the amino acids include 20 kinds of amino acids that construct proteins. In a case where DNA is used as a template, RNA polymerase is added to the reaction system, and a commercially available enzyme such as T7 RNA polymerase can be used.

The internal dialysate is put inside the dialysis membrane, and the external dialysate is put outside the membrane. By shaking or stirring of the closed system in which substances can transfer through the membrane in dependence on the cutoff molecular weight, a target protein thus produced can be collected from the internal or external dialysates. For the reaction conditions such as temperature, stirring rate, and so forth, any condition can be applied depending on the kind of proteins. In the case of protein synthesis, the temperature to be applied is usually approximately 25 to 50°C, preferably 37°C. However, the temperature for cell-free protein synthesis system using a fungus extract derived from *Thermus thermophilus* may exceed 50°C. Further, the shaking rate or stirring rate may be low, and, for example, 100 to 200 rpm can be applied. While observing the production of the target protein, the reaction period can be properly determined.

In the cell-free protein synthesis system, it is desirable to exchange the external dialysate for a fresh external dialysate when the reaction rate is reduced. Moreover, the use of a dialysis membrane with a cutoff molecular weight of more than 10,000 Da, preferably more than approximately 50,000 Da, enables higher output of the proteins.

[Purification of protein]

Since the quantity and the number of kinds of mixed contaminants are extremely small, compared with the isolation from living cells, purification of the produced proteins can be achieved with relative ease. Depending on the properties of the proteins, conventionally known purification methods can be used either alone or, if necessary, in combination. Common techniques can be used, such as ammonium sulfate or acetone precipitation, acid extraction, anion or cation exchange chromatography, hydrophobic interaction chromatography, affinity chromatography, gel filtration chromatography, HPLC, electrophoresis, and chromatofocusing.

During or after this purification process, a tag sequence used for purification can be removed by protease treatment. Identification and quantitative determination of the produced proteins can be achieved by activity assay, immunological assay, spectroscopic measurement, amino acid analysis, and the like, and, if necessary, comparing with a standard sample.

(Screening method)

As a screening method of the present invention, there is a method for screening a compound having interaction with a protein of the present invention, which comprises a process of bringing a candidate substance into contact with the protein or a salt thereof, and a process of confirming whether the protein interacts with the candidate substance. Here, the expression "having interaction" means to inhibit or strengthen molecular function and/or physiological activity of the protein by combining the compound with the protein and so on. In this screening method, the protein is brought into contact with the candidate substance, and it is determined whether molecular function or physiological activity of the protein is changed.

[Searching for an interactive substance using NMR]

When NMR is used to search for an interactive substance, the presence of interaction can be determined based on the existence of signal changes of the protein before and after addition of the candidate substance. In other words, when an

interactive candidate substance interacts with the protein, it is expected that a chemical shift value, a line width, the number, etc. of NMR signals derived from the vicinity of interactive site of the protein may be changed, and thus the presence of interaction can be determined by detecting such changes. In particular, ¹⁵N-labeled protein is prepared with relative ease, and ¹⁵N-HSQC spectrum obtained therefrom has relatively high resolution and sensitivity. Further, the spectrum is less affected by NMR signals derived from added interactive candidate substance, and thus it is very useful.

(Assay method)

The protein of the present invention can be assayed by using, for example, an antibody of the present invention. Examples of a method for assaying a protein using an antibody include sandwich immunoassay, competitive method, immunometric method, and nephelometry method. Further, it is also detectable using labels such as radioisotope, an enzyme, and a fluorescent material. (Screening method using assay method)

The antibody of the present invention is specifically combined with the protein of the present invention, and thus it can be used for screening a compound having interaction with the protein of the present invention. As a screening method therefor, known screening methods are usable.

In addition, according to the assay method of the protein of the present invention using the antibody of the present invention, diseases involving the protein of the present invention can be prevented and diagnosed.

(Three-dimensional structure analysis)

The three-dimensional structure of the protein can be analyzed by NMR structure analysis, X-ray structure analysis, etc.

(NMR)

A sample used for NMR is not particularly limited, but a sample in which ¹²C or ¹⁴N in the protein is labeled with a stable isotope, ¹³C or ¹⁵N nuclear is used preferably (multi-nuclear and multi-dimensional NMR measurement).

Stable-isotope labeling of a protein is a common technique, and is described in Clore, G.M.& Gronenborn, A.M., Science, 252, p.1390-1399, 1991, or the like. In particular, analysis using a protein sample having a main chain labeled with ¹⁵N uniform stable isotope is easily and preferably carried out. In addition, a protein having the skeleton of the main chain labeled with at least two or more kinds of isotopes of ¹³C, ¹⁵N, and ²H may be used (National Publication of International Patent Application No. 2001-514239).

It is preferable to measure ¹⁵N-¹H spin coupling constant by observing IPAP-HSQC spectrum, etc. The term "IPAP-HSQC spectrum" is a measurement method for reading ¹⁵N-¹H spin coupling constant effectively by simultaneously observing two HSQC spectra of level and reverse phases, and adding both spectra thereby to prevent overlapping of the signals.

Chemical shift attribution is performed by two or more kinds of NMR methods. For example, 2D, DOQ-COSY, TOCSY, NOESY, and HSQC are well known as two dimensional NMR, and HNCO, HCACO, HNCA, HCA(CO)N, HN(CO)CA, HNHB, CBCANH, H(CA)NH, HBHA(CO)NH, HCCH-COSY, HCANH, HCCH-TOCSY, HCACON, ¹⁵N-NOESY-HSQC, ¹³C-NOESY-HSQC are well known as multi dimensional NMR. A general technique of NMR is known, and described in, for example, "NMR of Protein" (Yoji Arata, Kyoritsu Shuppan, Co., Ltd., 1996); "Basic Biochemical Experiment Method Vol. 3, Protein I, Detection and Structure Analysis Method edited by Japan Biochemical Society" Chapter 18, Three-dimensional structure analysis by NMR (Tokyo Kagaku Dozin, Co., Ltd., Feb. 2001); Takashi Ito et al., Journal Vol. 21 of Japan Agrochemical Society, pp.

450-459, 1996; and Toshiyuki Tanaka, Chemistry and Industry Vol. 49, No. 2, pp. 155-158, 1996.

When NMR is used for three-dimensional structure analysis, it is a common method that the distance between protons is estimated in accordance with the scale of nucleus overhauser effect between individual protons of the protein, and based on the distance information, the three-dimensional structure is determined. It is possible to obtain a three-dimensional structure with precision by adding information concerning a chemical shift value, a scalar coupling value, a residual dipolar coupling value, hydrogen bond or the like.

Many programs for structure analysis from NMR data are known. Structure analysis is performed preferably by using NMR Pipe, PIPP, Capp, Felix, NMR View, and XEASY for chemical shift attribution, and by using X-PLOR, CNS, DYANA, and DYNAMO as three dimensional calculation softwares.

(X-ray crystallography)

When X-ray crystallography is used for three-dimensional structure analysis, an electron density map is calculated based on an X-ray diffraction image of crystallized protein, and the three-dimensional structure is determined. In other words, the protein is crystallized and mono-colored X-ray is applied to the crystal, and based on the obtained X-ray diffraction image, the three-dimensional structure of the protein is clarified (Blundell, T.L. and Johnson, L.N., PROTEIN CRYSTALLOGRAPHY, pp. 1-565, (1976) Academic Press, New York). (Screening method based on three-dimensional structure information)

Next, the present invention provides, using information concerning three-dimensional structure of the aforementioned protein, a method for screening a compound having interaction with the protein or a salt thereof, which comprises a process of determining an active site of the protein, and a process of searching for the compound having interaction with the active site on a computer.

(In silico screening)

Regarding drug design based on three-dimensional structure of a molecule, there are many reviews including Drug Development, Vol. 7 "Molecular Design" (Hirokawa Shoten). Specifically, screening is first conducted by a computer on the library (e.g. about 150,000 kinds) of low molecular compounds (1000 or less molecular weight) stored in a relational database such as Oracle by use of a flexible ligand binding simulation software such as FlexiDock and FlexX. The three-dimensional structure of a chemical compound of this library is designated by a program such as CONCORD, and it is possible to select a substance that can be inserted into an active site. Among the selected substances, a compound that is fit into the active site more precisely is visually selected by using a simulation program such as Insight II or MOE. Computer softwares used in a series of the above processes are the following commercially available ones.

FlexiDock: Tripos Inc.FlexX: Tripos Inc.CONCORD: Tripos Inc.Oracle: Oracle Corp.Insight II: Molecular Simulations Inc.MOE: Chemical Computing Group Inc.

Another method is to design candidate compounds including unknown substances by a computer. As such method, the following methods are known: a method for searching for a compatible compound by aligning a chemical group such as methyl and ethyl in an active site; and a method of aligning an atom in an active site by a computer program.

(Wet screening)

To select a major candidate compound having interaction with the protein of the present invention, the candidate compound obtained by in silico screening is brought into contact with the protein of the present invention and the molecular function or physiological activity of the protein of the invention is determined.

Based on the three-dimensional structure data of the candidate compound and the

protein of the invention, the candidate compound is modified so as to have more desirable structure.

The selected compound is synthesized and actually interacted with the protein for screening. With respect to a compound that has changed the activity of the protein, further testing relating to in vitro activity, in vivo dynamics, or toxicity is performed by animal tests.

(Pharmaceutical Agent containing an interactive substance)

A substance interacting with the protein of the invention can be used as a preventive and/or therapeutic agent to diseases involving the protein. Such a pharmaceutical agent can be orally or parenterally administered to the whole body or locally.

When the drug of the invention is orally administered, it may be prepared in any type of formulation such as a tablet, a capsule, a granule, powder, a pill, trochiscus, internal use liquor, a suspension, an emulsion, and syrup, and may be prepared as a dried product which is dissolved again at administration. Further, when the drug of the invention is parenterally administered, a formulation such as an intravenous injection (including intravenous drip), intramuscular injection, intraperitoneal injection, subcutaneous injection, and suppositories may be selected. In the case of formulations for injection, the drug may be provided in the form of an ample with a unit dose or a container for large volume administration.

These formulations can be produced by conventional methods by properly selecting an excipient, an extender, a binder, a wetting agent, a disintegrator, a lubricant, a surfactant, a dispersant, a buffer, a preservative, a solubilizing agent, an antiseptic, a corrective, an analgesic agent, a stabilizing agent, and an isotonic agent, which are commonly used for formulation.

The above various formulations may contain a pharmaceutically acceptable carrier or additive. Examples of these carriers and additives include water,

pharmaceutically acceptable organic solvents, collagen, polyvinyl alcohol, polyvinyl pyrrolidone, carboxyvinyl polymer, sodium alginate, water-soluble dextran, carboxymethyl starch sodium, pectin, xanthan gum, gum Arabic, casein, gelatin, agar, glycerol, propylene glycol, polyethylene glycol, Vaseline, paraffin, stearyl alcohol, stearic acid, a human serum albumin, mannitol, sorbitol, and lactose. Additives to be used are selected from the above-mentioned property or in combination according to the type of formulation of the invention.

A dose of the drug of the invention can be varied depending on the age of a recipient, administration path, and the number of administration times, and thus it can be changed in a wide range. In this case, the effective dose of the protein of the invention and the effective dose to be administered in combination with suitable diluent and pharmacologically usable carried are selected in the range of 0.01 mg to 1,000 mg per 1 kg of the body weight for one time, and the administration is conducted preferably once to several times per day for one day or more. (Description of Sequences)

The sequence numbers of the description indicate the following sequences.

SEQ ID NO:1 represents an amino acid sequence of a CAP-Gly like domain protein (KIAA0849 protein (464-554)).

SEQ ID NO:2 represents a DNA sequence encoding the protein of SEQ ID NO:1.

SEQ ID NO:3 represents an amino acid sequence of a CAP-Gly like domain protein (KIAA0849 protein (454-554)).

SEQ ID NO:4 represents a DNA sequence encoding the protein of SEQ ID NO:3.

SEQ ID NO:5 represents an amino acid sequence of a CAP-Gly like domain protein (KIAA0849 protein (454-559)) (amino acid sequence having amino acid

residues NTAPVQESPP and VSNQI added to the N- and C- terminals of the amino acid sequence of SEQ ID NO:1).

SEQ ID NO:6 represents a DNA sequence encoding the protein of SEQ ID NO:5.

SEQ ID NO:7 represents an amino acid sequence of a CAP-Gly like domain protein (KIAA0849 protein (464-559)).

SEQ ID NO:8 represents a DNA sequence encoding the protein of SEQ ID NO:7.

SEQ ID NO:9 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:10 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:11 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:12 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:13 represents a nucleotide sequence of a primer used for the following Example.

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SEQ ID NO:14 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:15 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:16 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:17 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:18 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:19 represents a nucleotide sequence of a primer used for the following Example.

SEQ ID NO:20 represents an amino acid sequence in which a plurality of amino acid residues are added to the N- and C- terminals of the amino acid sequence of SEQ ID NO:1.

SEQ ID NO:21 represents an amino acid sequence of IKK-gamma (1-419).

SEQ ID NO:22 represents a nucleotide sequence of cDNA of the protein represented by SEQ ID NO:21.

[Examples]

The present invention will be described in detail by showing Examples below, but the scope of the present invention is not limited by them.

[Example 1]

(1) Presumption of domain

The presumption of a domain was conducted in the following manner.

- First, 1) <SCOP method> when a region having homology with a sequence contained in protein database SCOP (Version 1.55) was detected from query sequences, such region was predicted as a domain. BLASTP was used as homology detection method, and it was determined to be homologous when E-value had 0.1 or less hits.
- 2) <PFAM method> when a region having homology with a sequence profile contained in protein motif database PFAM (version 6.5) was detected from query sequences, such region was predicted as a domain. HMMER was used as homology detection method, and it was determined to be homologous when E-value had 0.1 or less hits.

- 3) <ProDom method> when a region having homology with any of consensus sequences contained in protein motif database ProDom (a version obtained through the Web January, 2001) was detected from query sequences, such region was predicted as a domain. BLASTP was used as homology detection method, and it was determined to be homologous when E-value had 0.1 or less hits.
- 4) <NR method> homology search on query sequences was conducted by BLASTP in protein sequence data set (NCBI-nr), and when E-value had 0.1 or less hits, such homologous regions were grouped and predicted as domain.
- 5) <PASS method> homology search on query sequences was conducted by BLASTP in protein sequence data set (NCBI-nr), and the frequency of detecting homology was calculated. Peaks and troughs were used to indicate high frequency parts and low frequency parts, and one peak was predicted as domain so that a trough part is a domain boundary.
- 6) <No Hit method> regions (residual regions) that were not detected as domain by using any of the above 1) to 5) methods were predicted as domain.
- 7) <Differential domain boundary setting method> regarding the above six domain predictions, when a hit region was overlapped, high priority was given to 1), and followed by 2), 3), 4), 5), and 6) in this order. When the deviation of the domain boundary includes 30 residues or more and such residues are present in more length in the N- or C-terminal side in accordance with definition by lower priority method, though a hit region was overlapped, such differential sequence was predicted as other domain.

Among domain regions presumed by any of the above methods, regions having one or more Low-Complexity regions (sequence region with low complexity) or having the full length of less than 30 residues were removed.

Regarding the amino acid sequence of KIAA0849 protein, the presumption of domain region was conducted in the above-mentioned manner. According to NR

method, the range of 496th to 539th of amino acid residues was presumed as domain region. This domain region had no Low-Complexity region (sequence region with low complexity) and has the full length of 30 or more residues. Hence, this region was finally considered a result of domain presumption by bioinformatics.

(2) Producing Constructs

With respect to the protein (here referred to as presumed domain) having amino acid sequence of 496 to 539 amino acid residues of this KIAA0849 protein, protein synthesis reaction was conducted using a cell-free protein synthesis system described below. Thereafter, the obtained sample was subjected to SDS gel electrophoresis by conventional method to examine protein expression status.

As a result, a protein of interest was not expressed from information concerning amino acid sequence of the presumed domain.

Therefore, using the amino acid sequence of the presumed domain as a standard, constructs were systematically produced by extending or shortening the domain boundary position of the presumed domain, relative to amino acid sequence of KIAA0849 protein, by addition or deletion of several residues at the N- and C-terminals, respectively.

In other words, using, for example, 496th amino acid residue of KIAA0849 protein as a standard, a pattern having 10 residues added to the N-terminal side and 10 residues deleted from the C-terminal side was prepared. Also, using 539th amino acid residue of KIAA0849 protein as a standard, a pattern having 5 residues deleted from the N-terminal side and 5 residues added to the C-terminal side was prepared.

Using the constructs thus produced, protein expression for individual patterns was performed and their expression statuses were evaluated by SDS gel electrophoresis.

[Example 1]

In this example, among constructs produced in the above manner, KIAA0849 protein (464-554): (SEQ ID No. 1) having a CAP-Gly like domain suitable for three-dimensional structure analysis was studied. Results of the study are described.

(1) Construction of expression vector

(i) First PCR

Using a recombinant *E. coli* culture solution containing a plasmid wherein cDNA (DDBJ accession No. AB020656.2) encoding KIAA0849 protein was cloned in a plasmid pBluescriptII SK+, PCR was performed by use of 5'-primer 1 (SEQ ID NO:14) and 3'-primer 1 (SEQ ID NO:15). The composition of the PCR reaction solution is shown in Table 1. The program followed a conventional PCR protocol.

[Table 1] Composition of reaction solution for first PCR

| Composition | Concentration | Amount | Final concentration |
|---|---------------|---------|---------------------|
| Template plasmid | (×1/10) | 3 μL | (×3/200) |
| 5'-primer 1 | 0.25 μΜ | 4 μL | 0.05 μΜ |
| 3'-primer 1 | 0.25 μΜ | 4 μL | 0.05 μΜ |
| dNTPs(Toyobo) | 2 mM | 2 μL | 0.2 mM |
| Expand HiFi buffer solution (containing 15 mM magnesium chloride) (Roche) | (10×) | 2 μL | (1×) |
| Sterile distilled water | | 4.85 μL | |
| DNA polymerase (Roche) | 3.5 U/μL | 0.15 μL | 0.02625 U/μL |
| Total amount | | 20 μL | |

(ii) Secondary PCR

Next, second PCR was performed using the first PCR product obtained in the foregoing reaction, 5'-primer 2 (SEQ ID NO:17) having His tag sequence in the downstream of T7 promoter sequence, 3'-primer 2 (SEQ ID NO:18) having a T7 terminator sequence, and universal primer-U2 (SEQ ID NO:19). The composition of the PCR reaction solution is shown in Table 2. The program was the same as the above first PCR.

[Table 2] Composition of reaction solution for second PCR

| Composition | Concentration | Amount | Final |
|------------------------------|---------------|---------|-----------------|
| | | | concentration |
| First PCR product (template) | (×1/5) | 5 μL | $(\times 1/20)$ |
| 5'-primer 2 | 2 μΜ | 0.5 μL | 0.05 μΜ |
| 3'-primer 2 | 2 μΜ | 0.5 μL | 0.05 μΜ |
| Universal primer U2 | 100 μΜ | 0.2 μL | 1 μΜ |
| dNTPs (Toyobo) | 2 mM | 2 μL | 0.2 mM |
| Expand HiFi buffer solution | | | |
| (containing 15 mM magnesium | (10×) | 2 μL | (1×) |
| chloride) (Roche) | | | |
| Sterile distilled water | | 9.65 μL | |
| DNA polymerase (Roche) | 3.5 U/μL | 0.15 μL | 0.02625 U/μL_ |
| Total amount | | 20 μL | |

As a result, a linear double stranded DNA fragment was amplified, which can express a fusion protein of His tag sequence and KIAA0849 protein (464-554) under the control of T7 promoter.

(iii) Cloning

The DNA fragment obtained by the above second PCR reaction was cloned in a vector pPCR2.1 (Invtrogen) with TOPO TA-cloning kit (Invtrogen), and thereby an expression vector P011213-03 was constructed.

- (2) Expression of KIAA0849 protein (464-554)
- (i) Synthesis of ¹⁵N-labeled CAP-Gly-like domain by cell-free protein synthesis method using dialysis

E. coli S30 extract was prepared from E. coli BL21 codon plus strain according to a method of Zubay et al. (Annu. Rev. Geneti. 7, 267-287, 1973).

The protein synthesis reaction was conducted overnight at 30°C in the scale of 3 mL of reaction solution having the composition of Table 3 and 30 mL of external dialysate having the composition of Table 4.

[Table 3] Composition of reaction solution

| Composition | Final |
|--------------------|---------------|
| Composition | concentration |
| Hepes-KOH (pH 7.5) | 58 mM |

| DTT | 1.8 mM |
|---|-------------|
| ATP | 1.2 mM |
| CTP | 0.8 mM |
| GTP | 0.8 mM |
| UTP | 0.8 mM |
| Creatine phosphate | 80 mM |
| Creatine kinase | 0.25 mg/mL |
| Polyethylene glycol (average molecular weight 8000) | 4.0% |
| 3',5'-cAMP | 0.64 mM |
| L(-)-5-formyl-5,6,7,8-tetrahydroforic acid | 68 μM |
| E. coli total tRNA | 175 μg/mL |
| Potassium glutamate | 210 mM |
| Ammonium acetate | 27.5 mM |
| Magnesium acetate | 10.7 mM |
| [¹⁵ N] labeled amino acid mixture | 3 mg/mL |
| L-[¹⁵ N] cystein | 1 mM |
| L-[¹⁵ N] tryptophan | 1 mM |
| L-[¹⁵ N] glutamine | 1 mM |
| L-[¹⁵ N] asparagine | 1 mM |
| Sodium azide | 0.05% |
| T7 RNA polymerase | 66.6 μg/mL |
| S30 extract | 30% |
| Template DNA (P011213-03) | 1 μg/mL |

[Table 4] Composition of external dialysate

| Composition | Final |
|---|---------------|
| Composition | concentration |
| Hepes-KOH (pH 7.5) | 58 mM |
| DTT | 1.8 mM |
| ATP | 1.2 mM |
| CTP | 0.8 mM |
| GTP | 0.8 mM |
| UTP | 0.8 mM |
| Creatine phosphate | 80 mM |
| Creatine kinase | 0.25 mg/mL |
| Polyethylene glycol (average molecular weight 8000) | 4.0% |
| 3',5'-cAMP | 0.64 mM |
| L(-)-5-formyl-5,6,7,8-tetrahydroforic acid | 68 μM |
| Potassium glutamate | 210 mM |
| Ammonium acetate | 27.5 mM |
| Magnesium acetate | 10.7 mM |
| [15N]-labeled amino acid mixture | 3 mg/mL |
| L-[¹⁵ N] cystein | 1 mM |
| L-[¹⁵ N] trypptophan | 1 mM |
| L-[¹⁵ N] glutamine | 1 mM |
| L-[¹⁵ N] asparagine | 1 mM |

(ii) Determination of expression status by SDS gel electrophoresis

After the termination of the synthesis reaction, SDS gel electrophoresis was performed by a conventional method, and the expression status of the obtained protein was determined.

Results thereof are shown in Fig. 1A. According to Fig. 1A, it was confirmed that KIAA0849 protein (464-554) (CAP-Gly-like domain protein having an amino acid sequence represented by SEQ ID NO:1) was expressed. In Fig. 1A, the first lane is a lane of a protein containing a fraction of interest in purification, and M is a marker lane.

[Examples 2 to 4]

In Examples 2 to 4, among constructs produced in the above manner, KIAA0849 protein (454-554) (Example 2), KIAA0849 protein (454-559) (Example 3), and KIAA0849 protein (464-559) (Example 4) were studied. Results of the study are described.

Specifically, primers used for the first and second PCRs of Example 1 were changed to those shown in Table 5 and except that, an expression vector was constructed in the same manner as Example 1. The obtained linear double stranded DNA fragment was used as a template DNA for protein synthesis.

| [Table 5] | Sequence | numbers of | each | primer | used for | first and | second PCRs |
|-----------|----------|------------|------|--------|----------|-----------|-------------|
|-----------|----------|------------|------|--------|----------|-----------|-------------|

| | First PCR | | Second PCR | | | | |
|-------------|--------------|-----------------|-----------------|-----------------|------------------|--|--|
| Example No. | 5'-primer 1 | 3'-primer 1 | 5'-primer 2 | 3'-primer 2 | Universal primer | | |
| 1 | SEQ ID | SEQ ID | SEQ ID | SEQ ID | SEQ ID | | |
| | NO:14 | NO:15 | NO:17 | NO:18 | NO:19 | | |
| 2 | SEQ ID NO:13 | SEQ ID NO:15 | SEQ ID NO:17 | SEQ ID NO:18 | SEQ ID NO:19 | | |
| 3 | SEQ ID | SEQ ID | SEQ ID | SEQ ID | SEQ ID | | |
| | NO:13 | NO:16 | NO:17 | NO:18 | NO:19 | | |
| 4 | SEQ ID | SEQ ID | SEQ ID | SEQ ID | SEQ ID | | |
| | NO:14 | NO:16 | NO:17 | NO:18 | NO:19 | | |

After the termination of the synthesis reaction, SDS gel electrophoresis was performed in the same manner as in Example 1 to determine the expression level of the obtained proteins.

Results thereof are shown in Fig. 1B to Fig. 1D. Fig. 1B shows an SDS gel electrophoregram of Example 2, Fig. 1C shows an SDS gel electrophoregram of Example 3, and Fig. 1D shows an SDS gel electrophoregram of Example 4. In Figs. 1B to 1D, the first lane is a lane of a protein containing a fraction of interest in purification, and M is a marker lane, respectively. In Fig. 1B, a band is observed at a position corresponding to KIAA0849 protein (454-554). According to this result, it is found that KIAA0849 protein (454-554) was expressed in Example 2. Further, according to Fig. 1C, it was found that KIAA0849 protein (454-559) was expressed in Example 3 in the same way as Fig. 1B. Furthermore, according to Fig. 1D, it was found that KIAA0849 protein (464-559) was expressed in Example 4.

[Comparative Examples 1 to 3]

Among constructs produced in the above manner, expression vectors were constructed, using a similar way as described in the above Example 1, regarding polypeptide a (comparative example 1) having an amino acid sequence of 474th to 539th amino acid residues of KIAA0849 protein, polypeptide b (comparative

example 2) having an amino acid sequence of 454th to 539th amino acid residues, and polypeptide c (comparative example 3) having an amino acid sequence of 454th to 549th amino acid residues. The obtained linear double stranded DNA fragments were used as template DNAs for protein synthesis. At this time, instead of primers used for the first PCR in Example 1, primers of amino acid sequence properly designed for these comparative examples were used.

Then, the expression levels of the obtained samples were determined by SDS gel electrophoresis. Fig. 2 shows SDS gel electrophoregrams in comparative examples. Fig. 2A shows an SDS gel electrophoregram of comparative example 1, Fig. 2B shows an SDS gel electrophoregram of comparative example 2, and Fig. 2C shows an SDS gel electrophoregram of comparative example 3. Here, the first lane is a lane of the entire products, the second lane is a lane of a supernatant, and M is a marker lane, respectively.

In Fig. 2A, there appeared no band at a position of MW=11.1 kDa, a molecular weight estimated based on the amino acid sequence of polypeptide a. Therefore, according to Fig. 2A, it was found that a protein of interest was not expressed in comparative example 1.

Further, in Fig. 2B, there appeared no band at a position of 13.1 kDa, which is a molecular weight estimated based on the amino acid sequence of polypeptide b.

According to Fig. 2B, it was therefore found that a protein of interest was not expressed in comparative example 2.

Next, in Fig. 2C, a band appeared at an upper position from the position corresponding to 14.2 kDa, which is a molecular weight estimated based on the amino acid sequence of polypeptide c. According to Fig. 2C, it was thus found that a protein of interest was not obtained on a good expression level.

[Example 5]

With respect to respective proteins of interest in the above Examples 1 to 4 (proteins represented by SEQ ID NOS:1, 3, 5 and 7, respectively) were evaluated in terms of structural stability.

(1)Purification of ¹⁵N labeled domain

The proteins of interest synthesized in the above Examples 1 to 4 were purified.

To purify ¹⁵N labeled domain protein, the affinity of histidine tag and nickel was utilized. The operation was conducted at 4°C. First, after the termination of synthesis reaction, 3 ml of the reaction solution was diluted with 4.2 ml of washing buffer solution [50 mM sodium phosphate (pH 8.0)/300 mM sodium chloride/10 mM imidazole], collected and centrifuged at 1960 g for 5 minutes to remove precipitates. Next, the obtained supernatant was passed through 0.8 ml of Ni-NTA resin (QIAGEN) for adsorption, and passed through 9.6 ml of washing buffer solution to thereby remove contaminants. Finally, the resultant product was passed through 4 ml of elution buffer solution [50 mM sodium phosphate (pH 8.0)/300 mM sodium chloride/500 mM imidazole], and thereby the sample was liberated from the resin. According to the above procedures, 0.88 mg of purified sample was obtained.

(2) Sample preparation for structural stability evaluation

To make the purified sample a solvent suitable for NMR measurement, substitution by 20 mM sodium phosphate (pH 6.0)/100 mM sodium chloride solution was conducted. Thereafter, the sample was concentrated to 0.25 ml (sample concentration: 0.28 mM). For the above operations, an ultrafilter (VIVASPIN 2; SARTORIUS) was used. Finally, 0.03 ml of heavy water was added, thereby obtaining a sample for structural stability evaluation.

(3)Structural stability evaluation by NMR measurement

As a sample tube for NMR measurement, a symmetrical microtube (for 5 mm probe) manufactured by Shigemi, Inc. was used. The NMR measurement was conducted by a 600 MHz-NMR instrument (Avance 600 manufactured by Bruker) at 25°C. For the evaluation, one-dimensional spectrum of ¹H (hereinafter abbreviated as 1D spectrum), and ¹H-¹⁵N two-dimensional HSQC spectrum (hereinafter abbreviated as ¹⁵N-HSQC spectrum) were used, and the conditions therefor were shown in the table 6 below. The results of the NMR measurement are shown in the figures 3 to 6.

[Table 6] NMR measurement conditions for structural stability evaluation

| Spectrum | Accumulated times | Center frequency | Spectrum width | Data point number |
|-------------|-------------------|---|---|--|
| 1D | 128 | ¹ H: 2822 Hz | ¹ H: 8013 Hz | ¹ H: 8192 |
| T5N HSQC | 16 | ¹ H: 2822 Hz ¹⁵ N: 7085 Hz | ¹ H: 8013 Hz ¹⁵ N: 2190 Hz | ¹ H: 2048 ¹⁵ N: 128 |

Figs. 3 to 6 show one-dimensional nuclear magnetic resonance spectra and $^{1}\text{H}-^{15}\text{N}$ HSQC spectra of the proteins represented by SEQ ID NOS:1, 3, 5 and 7, respectively. In Figs. 3 to 6, figure A shows a one-dimensional nuclear magnetic resonance spectrum, and figure B shows a $^{1}\text{H}-^{15}\text{N}$ HSQC spectrum.

In Figs. 3A to 6A, signals shifted to higher magnetic field were recognized at a higher magnetic field side (around 0.7 ppm to -0.5 ppm) in the methyl region of one-dimensional nuclear magnetic resonance spectra. In Figs. 3B to 6B, signals of removed amide proton were recognized at a range of 7 ppm to 9 ppm in ¹⁵N HSQC spectra.

Since the appearance of these signals is characteristic to a protein forming a stable three-dimensional structure, it was determined that the proteins obtained in the above examples 1 to 4 formed a stable three-dimensional structure.

In the examples 1 to 4, as mentioned above, amino acid sequences of constituent element (domain) having structure and function of a protein were predicted from full-length KIAA0849 protein by a computer, and all constructs of various kinds were produced on the basis of the predicted region for protein expression. The expression statuses of the actually obtained proteins were confirmed by SDS gel electrophoresis. Then, whether or not they have a stable three-dimensional structure was evaluated by NMR measurement, and all the proteins were confirmed to have excellent structural stability.

Therefore, according to the examples, it has been confirmed that an amino acid sequence of CAP-Gly-like domain having actually stable three-dimensional structure (folding) was correctly determined.

Moreover, use of such domain-forming protein having a small molecular weight enables highly accurate three-dimensional structure analysis with relative ease.

Then, using KIAA0849 protein (464-554) of Example 1 that is a CAP-Gly-like domain protein having an amino acid sequence represented by SEQ ID NO:1, the three-dimensional structure analysis was conducted as follows.

[Example 6]

Structure determination of CAP-Gly-like domain protein contained in cancer suppressor gene (KIAA0849) product involved in human Turban tumor syndrome

(1) Purification of ¹³C¹⁵N-labeled domain by NMR measurement

A protein represented by SEQ ID NO:20 having all the carbon and nitrogen nuclears substituted by stable isotope carbon 13 and nitrogen 15 was produced by the above cell-free protein expression system. The protein represented by SEQ ID NO:20 is a protein derived from the protein represented by SEQ ID NO:1 by addition of amino acid residues represented by GSSGSSG and SGPSSG to the N- and

C-terminals, and these additional sequences do not affect three-dimensional structure of the protein. Therefore, analysis of three-dimensional structure of the protein represented by SEQ ID NO:20 provides three-dimensional structure of the protein of the present invention represented by SEQ ID NO:1.

The obtained high purity preparation was concentrated to a standard concentration of 0.8 mM using a protein concentrator with an ultrafilter membrane for a high-speed centrifuge, and thereafter diluted 10 times with preparation buffer solution for NMR analysis. These concentration and dilution processes were repeated three times, and the buffer solution for purifying preparation was completely substituted by the preparation buffer solution for NMR analysis. The used preparation buffer solution for NMR analysis was composed of 20 mM sodium phosphate, 100 mM sodium chloride, 1 mM dithiothreitol, and pH thereof was 6.0. After complete substitution by the preparation buffer solution for NMR analysis, the final concentration of the preparation was about 0.8 mM. The obtained preparation was injected to a test tube for NMR measurement with an outer diameter of 5 mm, and then preserved at 25°C for 2 hours for stabilization.

(2) NMR measurement

For NMR experiment, DRX600 and DRX800 manufactured by Swiss Bruker were used. All the measurements were conducted at 25°C. In NMR experiment having a purpose of main chain signal attribution, a two dimensional spectrum of ¹H-¹⁵N HSQC, and three dimensional spectrum of HNCO, HN(CO)CA, HNCA, CBCA(CO)NH, HNCACB, HBHA(CBCACO)NH, H(CCCO)NH, C(CCCO)NH, and ¹⁵N-edited NOESY were measured. In addition, in NMR experiment having a purpose of side chain signal attribution, two dimensional spectrum of ¹H-¹³C HSQC and three dimensional spectra: HCCH-COSY, HCCH-TOCSY, ¹³C-edited NOESY for aliphatic side chain; and HCCH-COSY, ¹³C-edited NOESY, HNHB, and HN(CO)HB for aromatic side chain were measured.

(3) Analysis of measurement data

The measurement data were subjected to Fourier transform using work stations Octane2 and Origin3800 manufactured by Silicon Graphics, Inc. in America, and respective two dimensional and three dimensional spectra were obtained. Based on the obtained spectrum data, $C\alpha$ and $C\beta$ of carbon nuclear at α and β positions as main chain signals of amino acid residue; C' of carbon nuclear of carbonyl group; H α and H β of hydrogen nuclear at α and β positions; HN of hydrogen nuclear of amino group; and N of nitrogen nuclear of amide group were attributed in a chain reaction manner. In this method, a signal having a chemical shift value identical to that of Ca signal of an adjacent residue on HN(CO)Ca was searched for on HNCA, and the linkage with Ca signal of a residue adjacent to itself was clarified. This process was repeated, and thereby all $C\alpha$ signals were attributable in a chain reaction manner, except that signals were not observed due to proline residue or from any cause. By conducting the same procedure, CB signals by C(CCCO)NH. CBCA(CO)NH, and HNCACB, Hα and Hβ signals by H(CCCO)NH, HBHA(CBCACO)NH and ¹⁵N-edited NOESY, and C' signals by HNCO were attributed, and thereby more precise attribution can be conducted. Further, using the obtained spectrum data measured for main chain attribution information and side chain attribution, attributions of carbon, nitrogen, and hydrogen nuclears at γ , δ , ϵ , ζ , and η positions were conducted. According to the above procedures, attribution data of signals regarding to almost all the amino acid residues was obtained. Moreover, distance limitation data was obtained from 1142 signals on ¹⁵N-edited NOESY, 2158 signals on ¹³C-edited NOESY for aliphatic side chain, and 209 signals on ¹³C-edited NOESY for aromatic side chain. From the chemical shift values, obtained during main chain attribution, of Cα, Cβ, C', Hα, Hβ, HN, and N signals, ϕ and ψ angle data of 42 residues were obtained using a software TALOS, which predicted with high precision ϕ and ψ angles, dihedral angles of polypeptide

main chain. Furthermore, according to signal patterns of HNHB and HN(CO)HB, data of χ angle, which was a dihedral angle of side chain in 35 residues was obtained. Based on these signal attribution data, distance limitation data, ϕ , ψ , and χ angle limit data, a domain structure was calculated using CNS, a software for protein three-dimensional structure calculation. Based on the obtained three-dimensional structure, NOE group which did not meet provided distance limit was compared and reviewed, and then optimized. This process was repeated, and finally calculation was conducted using all the angle limits and 2667 distance limits, thereby obtaining 20 energetically stable three-dimensional structures. In these structures, the convergence of amino acid residues forming two dimensional structure was 0.29 Å relative to atom group of main chains and 0.76 Å relative to all atom group including side chains except hydrogen atom.

(4) Structure coordinates

Structure coordinates are shown in the following three-dimensional structure coordinate tables 1 to 20.

The following three-dimensional structure coordinate data is described in accordance with the format of protein data bank (PDB). ATOM of the first column indicates that this column is a column for atomic coordinate; the second column indicates the order of atoms; the third column indicates the distinction of atom in amino acid residues, etc.; the fourth column indicates amino acid residues, etc.; the fifth column indicates the number of amino acid corresponding SEQ ID NO:20; the sixth, seventh, and eighth columns indicate coordinates of atom (unit: Å, in the order of a, b and c axes); the ninth column indicates occupancy of that atom (anytime this figure is 1.00 in the invention); the tenth column indicates temperature factor of that atom. The final line indicates the final line of this table.

Three-Dimensional Structure Coordinate Table 1

| ATOM 1 | N | GLY A | 1120.138 | 11.140 | -2.903 | 1.00 | 0.00 N |
|----------|-----|-------|----------|--------|---------|------|--------|
| ATOM 2 | CA | GLY A | 1120.658 | 10.305 | -1.785 | 1.00 | 0.00 C |
| ATOM 3 | C | GLY A | 1120.202 | 8.862 | -1.879 | 1.00 | 0.00 C |
| ATOM 4 | О | GLY A | 1119.025 | 8.590 | -2.119 | 1.00 | 0.00 O |
| ATOM 5 1 | Н | GLY A | 1120.758 | 11.050 | -3.733 | 1.00 | 0.00 H |
| ATOM 62 | Н | GLY A | 1120.103 | 12.139 | -2.617 | 1.00 | 0.00 H |
| ATOM 7 3 | Н | GLY A | 1119.180 | 10.832 | -3.164 | 1.00 | 0.00 H |
| ATOM 8 1 | HA | GLY A | 1121.737 | 10.331 | -1.802 | 1.00 | 0.00 H |
| ATOM 9 2 | HA | GLY A | 1120.312 | 10.720 | -0.850 | 1.00 | 0.00 H |
| ATOM10 | N | SER A | 2121.135 | 7.935 | -1.688 | 1.00 | 0.00 N |
| ATOM11 | CA | SER A | 2120.822 | 6.512 | -1.752 | 1.00 | 0.00 C |
| ATOM12 | C | SER A | 2119.883 | 6.109 | -0.621 | 1.00 | 0.00 C |
| ATOM13 | О | SER A | 2119.959 | 6.647 | 0.484 | 1.00 | 0.00 O |
| ATOM14 | СВ | SER A | 2122.107 | 5.683 | -1.684 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2122.628 | 5.441 | -2.980 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2122.055 | 8.214 | -1.500 | 1.00 | 0.00 H |
| ATOM17 | HA | SER A | 2120.333 | 6.322 | -2.695 | 1.00 | 0.00 H |
| ATOM18 | IНВ | SER A | 2122.846 | 6.217 | -1.107 | 1.00 | 0.00 H |
| ATOM19 2 | 2HB | SER A | 2121.896 | 4.735 | -1.211 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2122.628 | 6.259 | -3.482 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3118.997 | 5.160 | - 0.902 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3118.042 | 4.685 | 0.092 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3118.645 | 3.564 | 0.933 | 1.00 | 0.00 C |
| ATOM24 | O | SER A | 3118.658 | 2.404 | 0.523 | 1.00 | 0.00 O |
| ATOM25 | СВ | SER A | 3116.764 | 4.194 | -0.591 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3117.063 | 3.463 | -1.768 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3118.986 | 4.769 | -1.801 | 1.00 | 0.00 H |

| ATOM28 | НА | SER A | 3117.798 | 5.513 | 0.739 | 1.00 | 0.00 H |
|--------|-----|-------|----------|-------|--------|------|--------|
| ATOM29 | 1HB | SER A | 3116.220 | 3.553 | 0.087 | 1.00 | 0.00 H |
| ATOM30 | 2HB | SER A | 3116.152 | 5.044 | -0.854 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3117.138 | 4.068 | -2.510 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4119.143 | 3.920 | 2.114 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4119.741 | 2.933 | 2.993 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4119.727 | 3.367 | 4.446 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4118.924 | 4.213 | 4.840 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4119.105 | 4.860 | 2.388 | 1.00 | 0.00 H |
| ATOM37 | 1HA | GLY A | 4119.195 | 2.005 | 2.901 | 1.00 | 0.00 H |
| ATOM38 | 2HA | GLY A | 4120.764 | 2.767 | 2.689 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5120.616 | 2.785 | 5.244 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5120.703 | 3.116 | 6.662 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5122.050 | 3.754 | 6.990 | 1.00 | 0.00 C |
| ATOM42 | О | SER A | 5122.125 | 4.697 | 7.777 | 1.00 | 0.00 O |
| ATOM43 | CB | SER A | 5120.499 | 1.861 | 7.513 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5119.829 | 2.169 | 8.723 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5121.230 | 2.118 | 4.870 | 1.00 | 0.00 H |
| ATOM46 | HA | SER A | 5119.919 | 3.824 | 6.886 | 1.00 | 0.00 H |
| ATOM47 | 1HB | SER A | 5119.907 | 1.147 | 6.961 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5121.461 | 1.428 | 7.747 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5120.475 | 2.376 | 9.402 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6123.109 | 3.233 | 6.381 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6124.454 | 3.751 | 6.607 | 1.00 | 0.00 C |
| ATOM52 | C · | SER A | 6124.821 | 4.789 | 5.552 | 1.00 | 0.00 C |
| ATOM53 | О | SER A | 6124.732 | 4.528 | 4.353 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6125.472 | 2.611 | 6.594 | 1.00 | 0.00 C |

| ATOM55 | OG | SER A | 6126.514 | 2.846 | 7.526 | 1.00 | 0.00 O |
|--------|------|-------|----------|-------|-------|------|--------|
| ATOM56 | Н | SER A | 6122.985 | 2.481 | 5.763 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6124.467 | 4.223 | 7.579 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6124.978 | 1.686 | 6.853 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6125.901 | 2.525 | 5.606 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6126.892 | 2.007 | 7.803 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7125.235 | 5.968 | 6.007 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7125.610 | 7.027 | 5.088 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7127.112 | 7.214 | 5.001 | 1.00 | 0.00 C |
| ATOM64 | O | GLY A | 7127.869 | 6.243 | 5.033 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7125.286 | 6.119 | 6.974 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7125.230 | 6.788 | 4.107 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7125.161 | 7.951 | 5.421 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8127.545 | 8.467 | 4.889 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8128.966 | 8.780 | 4.795 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8129.559 | 8.221 | 3.505 | 1.00 | 0.00 C |
| ATOM71 | O | LEU A | 8130.682 | 7.717 | 3.493 | 1.00 | 0.00 O |
| ATOM72 | CB | LEU A | 8129.719 | 8.220 | 6.004 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8129.030 | 8.435 | 7.352 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8129.288 | 7.256 | 8.279 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8129.506 | 9.731 | 7.991 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8126.893 | 9.197 | 4.867 | 1.00 | 0.00 H |
| ATOM77 | HA | LEU A | 8129.068 | 9.855 | 4.786 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8129.853 | 7.157 | 5.856 | 1.00 | 0.00 H |
| ATOM79 | 2HB | LEU A | 8130.692 | 8.685 | 6.043 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8127.964 | 8.510 | 7.196 | 1.00 | 0.00 H |
| ATOM81 | 1HD1 | LEU A | 8129.004 | 7.522 | 9.286 | 1.00 | 0.00 H |

| ATOM82 21 | HD1 | LEU A | 1 | 8130. | 337 | 7.002 | 8 | 3.254 | 1.00 | 0.00 F | ł |
|-----------|-----|-------|----|-------|-------|--------|------|--------|--------|--------|--------|
| ATOM83 31 | HD1 | LEU A | 1 | 8128. | 704 | 6.408 | - | 7.952 | 1.00 | 0.00 F | I |
| ATOM84 11 | HD2 | LEU A | 1 | 8130. | 301 | 9.516 | 8 | 3.691 | 1.00 | 0.00 F | ł |
| ATOM85 21 | HD2 | LEU A | 1 | 8128. | 684 | 10.199 | 8 | 3.512 | 1.00 | 0.00 F | H · |
| ATOM86 31 | HD2 | LEU A | 1 | 8129. | 872 | 10.397 | 7 | 7.224 | 1.00 | 0.00 F | I |
| ATOM87 | N | ALA | A | 9128 | .795 | 8.314 | 1 | 2.423 | 1.00 | 0.00 | N |
| ATOM88 | CA | ALA | A | 9129 | 9.241 | 7.81 | 8 | 1.128 | 1.00 | 0.00 | C |
| ATOM89 | C | ALA | A | 9129 | .592 | 8.968 | 3 | 0.192 | 1.00 | 0.00 | C . |
| ATOM90 | О | ALA | A | 9128 | .799 | 9.890 |) | 0.000 | 1.00 | 0.00 | O |
| ATOM91 | СВ | ALA | Α | 9128 | 3.171 | 6.93 | 4 | 0.504 | 1.00 | 0.00 | C |
| ATOM92 | Н | ALA | A | 9127 | .908 | 8.725 | 5 | 2.497 | 1.00 | 0.00 | Н |
| ATOM93 | HA | ALA | Α | 9130 | 0.123 | 7.21 | 6 | 1.289 | 1.00 | 0.00 | Н |
| ATOM94 1 | НВ | ALA | A | 9127 | .782 | 6.258 | 3 | 1.251 | 1.00 | 0.00 | Н |
| ATOM95 2 | HB | ALA | A | 9128 | .602 | 6.365 | 5 - | 0.308 | 1.00 | 0.00 H | Η . |
| ATOM96 3 | НВ | ALA | A | 9127 | .369 | 7.552 | 2 | 0.126 | 1.00 | 0.00 | Н |
| ATOM97 | N | MET | A | 10130 | 0.785 | 8.90 | 8 - | 0.389 | 1.00 | 0.00 | N |
| ATOM98 | CA | MET | Α | 1013 | 1.242 | 9.94 | 5 . | -1.306 | 1.00 | 0.00 | C |
| ATOM99 | C | MET | A | 10131 | .920 | 9.33 | 1 - | 2.528 | 1.00 | 0.00 | С |
| ATOM | 100 | O | ME | TΑ | 1013 | 3.135 | 9.4 | 142 - | -2.697 | 1.00 | 0.00 O |
| ATOM | 101 | CB | MF | ET A | 1013 | 2.206 | 10. | 896 | -0.594 | 1.00 | 0.00 C |
| ATOM | 102 | CG | MI | ET A | 1013 | 1.568 | 11. | 663 | 0.553 | 1.00 | 0.00 C |
| ATOM | 103 | SD | ME | ETA | 1013 | 2.377 | 13. | 245 | 0.863 | 1.00 | 0.00 S |
| ATOM | 104 | CE | ME | ETA | 1013 | 2.247 | 14. | 013 | -0.751 | 1.00 | 0.00 C |
| ATOM | 105 | Н | ME | ETA | 1013 | 1.373 | 8. | 148 - | -0.197 | 1.00 | 0.00 H |
| ATOM | 106 | HA | MI | ET A | 1013 | 30.376 | 10. | 503 | -1.632 | 1.00 | 0.00 H |
| ATOM | 107 | 1HB | ME | TA | 1013 | 3.031 | 10.3 | 321 - | -0.200 | 1.00 | 0.00 H |
| ATOM | 108 | 2HB | ME | TA | 1013 | 2.585 | 11.6 | 509 - | 1.310 | 1.00 | 0.00 H |
| | | | | | | | | | | | |

| ATOM | 109 1 | HG | MET A | 10130.531 | 11.846 | 0.314 | 1.00 | 0.00 H |
|--------|-------|-----|-------|-----------|--------|---------|------|--------|
| ATOM | 110 2 | HG | MET A | 10131.629 | 11.062 | 1.448 | 1.00 | 0.00 H |
| ATOM | 111 1 | HE | MET A | 10133.228 | 14.073 | -1.200 | 1.00 | 0.00 H |
| ATOM | 112 2 | HE | MET A | 10131.839 | 15.007 | -0.644 | 1.00 | 0.00 H |
| ATOM | 113 3 | HE | MET A | 10131.598 | 13.422 | -1.380 | 1.00 | 0.00 H |
| ATOM | 114 | N | PRO A | 11131.139 | 8.673 | -3.402 | 1.00 | 0.00 N |
| ATOM | 115 | CA | PRO A | 11131.671 | 8.043 | -4.613 | 1.00 | 0.00 C |
| ATOM | 116 | C | PRO A | 11132.451 | 9.024 | -5.486 | 1.00 | 0.00 C |
| ATOM | 117 | О | PRO A | 11133.544 | 8.709 | -5.957 | 1.00 | 0.00 O |
| ATOM | 118 | СВ | PRO A | 11130.423 | 7.547 | -5.350 | 1.00 | 0.00 C |
| ATOM | 119 | CG | PRO A | 11129.365 | 7.447 | -4.304 | 1.00 | 0.00 C |
| ATOM | 120 | CD | PRO A | 11129.682 | 8.497 | - 3.277 | 1.00 | 0.00 C |
| ATOM | 121 | НА | PRO A | 11132.304 | 7.202 | -4.372 | 1.00 | 0.00 H |
| ATOM | 122 1 | ΙНВ | PRO A | 11130.152 | 8.253 | -6.120 | 1.00 | 0.00 H |
| ATOM | 123 2 | ΣНВ | PRO A | 11130.626 | 6.585 | -5.795 | 1.00 | 0.00 H |
| ATOM | 124 | HG | PRO A | 11128.400 | 7.638 | -4.744 | 1.00 | 0.00 H |
| ATOM | 125 2 | 2HG | PRO A | 11129.387 | 6.466 | -3.855 | 1.00 | 0.00 H |
| ATOM | 126 | IHD | PRO A | 11129.162 | 9.416 | -3.504 | 1.00 | 0.00 H |
| ATOM | 127 2 | 2HD | PRO A | 11129.421 | 8.149 | -2.288 | 1.00 | 0.00 H |
| ATOM | 128 | N | PRO A | 12131.907 | 10.235 | -5.713 | 1.00 | 0.00 N |
| ATOM . | 129 | CA | PRO A | 12132.573 | 11.253 | -6.531 | 1.00 | 0.00 C |
| ATOM | 130 | C | PRO A | 12133.937 | 11.637 | -5.966 | 1.00 | 0.00 C |
| ATOM | 131 | O | PRO A | 12134.781 | 12.188 | -6.673 | 1.00 | 0.00 O |
| ATOM | 132 | CB | PRO A | 12131.618 | 12.453 | -6.477 | 1.00 | 0.00 C |
| ATOM | 133 | CG | PRO A | 12130.301 | 11.882 | -6.078 | 1.00 | 0.00 C |
| ATOM | 134 | CD | PRO A | 12130.613 | 10.712 | -5.191 | 1.00 | 0.00 C |
| ATOM | 135 | НА | PRO A | 12132.688 | 10.926 | -7.553 | 1.00 | 0.00 H |

| ATOM | 136 1HB | PRO A | 12131.975 | 13.167 | -5.750 | 1.00 | 0.00 H |
|------|----------|---------|-----------|--------|--------|------|--------|
| ATOM | 137 2HB | PRO A | 12131.566 | 12.918 | -7.451 | 1.00 | 0.00 H |
| ATOM | 138 1HG | PRO A | 12129.729 | 12.621 | -5.537 | 1.00 | 0.00 H |
| ATOM | 139 2HG | PRO A | 12129.761 | 11.555 | -6.954 | 1.00 | 0.00 H |
| ATOM | 140 1HD | PRO A | 12130.705 | 11.030 | -4.163 | 1.00 | 0.00 H |
| ATOM | 141 2HD | PRO A | 12129.854 | 9.952 | -5.287 | 1.00 | 0.00 H |
| ATOM | 142 N | GLY A | 13134.145 | 11.341 | -4.687 | 1.00 | 0.00 N |
| ATOM | 143 CA | GLY A | 13135.408 | 11.661 | -4.048 | 1.00 | 0.00 C |
| ATOM | 144 C | GLY A | 13136.522 | 10.720 | -4.461 | 1.00 | 0.00 C |
| ATOM | 145 O | GLY A | 13137.189 | 10.944 | -5.472 | 1.00 | 0.00 O |
| ATOM | 146 H | GLY A | 13133.435 | 10.900 | -4.171 | 1.00 | 0.00 H |
| ATOM | 147 1HA | GLY A | 13135.687 | 12.670 | -4.313 | 1.00 | 0.00 H |
| ATOM | 148 2HA | GLY A | 13135.282 | 11.603 | -2.977 | 1.00 | 0.00 H |
| ATOM | 149 N | ASN A | 14136.723 | 9.665 | -3.678 | 1.00 | 0.00 N |
| ATOM | 150 CA | ASN A | 14137.765 | 8.687 | -3.969 | 1.00 | 0.00 C |
| ATOM | 151 C | ASN A | 14137.162 | 7.396 | -4.514 | 1.00 | 0.00 C |
| ATOM | 152 O | ASN A | 14137.556 | 6.914 | -5.575 | 1.00 | 0.00 O |
| ATOM | 153 CB | ASN A | 14138.580 | 8.389 | -2.709 | 1.00 | 0.00 C |
| ATOM | 154 CG | ASN A | 14139.257 | 9.626 | -2.152 | 1.00 | 0.00 C |
| ATOM | 155 OD | l ASN A | 14140.304 | 10.048 | -2.643 | 1.00 | 0.00 O |
| ATOM | 156 ND | 2 ASN A | 14138.660 | 10.215 | -1.122 | 1.00 | 0.00 N |
| ATOM | 157 H | ASN A | 14136.159 | 9.542 | -2.887 | 1.00 | 0.00 H |
| ATOM | 158 HA | ASN A | 14138.418 | 9.109 | -4.718 | 1.00 | 0.00 H |
| ATOM | 159 1HB | ASN A | 14137.925 | 7.988 | -1.950 | 1.00 | 0.00 H |
| ATOM | 160 2HB | ASN A | 14139.341 | 7.660 | -2.944 | 1.00 | 0.00 H |
| ATOM | 161 1HD2 | ASN A | 14137.829 | 9.823 | -0.784 | 1.00 | 0.00 H |
| ATOM | 162 2HD2 | ASN A | 14139.076 | 11.018 | -0.744 | 1.00 | 0.00 H |
| | | | | | | | |

| ATOM | 163 | N | SER A | 15136.202 | 6.842 | -3.779 | 1.00 | 0.00 N |
|------|-----|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 164 | CA | SER A | 15135.544 | 5.607 | -4.189 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15134.436 | 5.233 | -3.208 | 1.00 | 0.00 C |
| ATOM | 166 | О | SER A | 15133.344 | 4.832 | -3.612 | 1.00 | 0.00 O |
| ATOM | 167 | СВ | SER A | 15136.561 | 4.468 | -4.286 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15137.099 | 4.375 | -5.592 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15135.930 | 7.274 | -2.943 | 1.00 | 0.00 H |
| ATOM | 170 | НА | SER A | 15135.106 | 5.770 | -5.163 | 1.00 | 0.00 H |
| ATOM | 171 | 1HB | SER A | 15137.366 | 4.649 | -3.590 | 1.00 | 0.00 H |
| ATOM | 172 | 2HB | SER A | 15136.076 | 3.535 | -4.041 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15136.766 | 3.582 | -6.020 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16134.726 | 5.365 | -1.919 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.756 | 5.041 | -0.879 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16134.196 | 5.603 | 0.468 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.479 | 6.389 | 1.089 | 1.00 | 0.00 O |
| ATOM | 178 | CB | HIS A | 16133.574 | 3.525 | -0.778 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16132.466 | 2.998 | -1.636 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16131.131 | 3.188 | -1.343 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16132.499 | 2.283 | -2.786 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16130.392 | 2.611 | -2.275 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16131.198 | 2.057 | -3.162 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16135.614 | 5.688 | -1.660 | 1.00 | 0.00 H |
| ATOM | 185 | HA | HIS A | 16132.814 | 5.491 | -1.153 | 1.00 | 0.00 H |
| ATOM | 186 | 1HB | HIS A | 16134.489 | 3.038 | -1.081 | 1.00 | 0.00 H |
| ATOM | 187 | 2HB | HIS A | 16133.355 | 3.264 | 0.247 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16130.779 | 3.672 | -0.567 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16133.384 | 1.952 | -3.310 | 1.00 | 0.00 H |

| ATOM | 190 | HE1 | HIS A | 16129.313 | 2.598 | -2.306 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|-------|--------|------|--------|
| ATOM | 191 | HE2 | HIS A | 16130.911 | 1.498 | -3.913 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.381 | 5.198 | 0.914 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17135.896 | 5.673 | 2.185 | 1.00 | 0.00 C |
| ATOM | 194 | C | GLY A | 17137.255 | 5.085 | 2.515 | 1.00 | 0.00 C |
| ATOM | 195 | О | GLY A | 17137.399 | 4.345 | 3.488 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.909 | 4.572 | 0.377 | 1.00 | 0.00 H |
| ATOM | 197 1 | НА | GLY A | 17135.981 | 6.748 | 2.148 | 1.00 | 0.00 H |
| ATOM | 198 2 | 2HA | GLY A | 17135.201 | 5.403 | 2.967 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18138.253 | 5.417 | 1.703 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.607 | 4.918 | 1.913 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.527 | 6.030 | 2.407 | 1.00 | 0.00 C |
| ATOM | 202 | O | LEU A | 18140.851 | 6.956 | 1.663 | 1.00 | 0.00 O |
| ATOM | 203 | СВ | LEU A | 18140.160 | 4.320 | 0.618 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18139.326 | 3.186 | 0.021 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18139.476 | 3.153 | -1.493 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18139.730 | 1.851 | 0.628 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18138.075 | 6.012 | 0.944 | 1.00 | 0.00 H |
| ATOM | 208 | НА | LEU A | 18139.562 | 4.144 | 2.665 | 1.00 | 0.00 H |
| ATOM | 209 1 | НВ | LEU A | 18140.234 | 5.111 | -0.115 | 1.00 | 0.00 H |
| ATOM | 210 2 | 2HB | LEU A | 18141.151 | 3.942 | 0.815 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18138.283 | 3.356 | 0.248 | 1.00 | 0.00 H |
| ATOM | 212 | HD1 | LEU A | 18139.372 | 2.136 | -1.842 | 1.00 | 0.00 H |
| ATOM | 213 2 | 2HD1 | LEU A | 18140.451 | 3.528 | -1.766 | 1.00 | 0.00 H |
| ATOM | 214 3 | 3HD1 | LEU A | 18138.713 | 3.768 | -1.944 | 1.00 | 0.00 H |
| ATOM | 215 | HD2 | LEU A | 18140.757 | 1.903 | 0.959 | 1.00 | 0.00 H |
| ATOM | 216 2 | 2HD2 | LEU A | 18139.629 | 1.073 | -0.113 | 1.00 | 0.00 H |

| ATOM | 2173 | 3HD2 | LEU A | 18139.092 | 1.630 | 1.471 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|-------|-------|------|--------|
| ATOM | 218 | N | GLU A | 19140.945 | 5.931 | 3.664 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.830 | 6.927 | 4.257 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19142.859 | 6.267 | 5.168 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19142.811 | 5.059 | 5.403 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19141.017 | 7.954 | 5.047 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.018 | 7.331 | 6.010 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19138.580 | 7.626 | 5.632 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19138.293 | 8.777 | 5.240 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19137.741 | 6.705 | 5.727 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.653 | 5.168 | 4.207 | 1.00 | 0.00 H |
| ATOM | 228 | НА | GLU A | 19142.347 | 7.431 | 3.454 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19141.696 | 8.573 | 5.617 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19140.474 | 8.579 | 4.353 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19140.161 | 6.261 | 6.013 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19140.202 | 7.721 | 7.000 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.791 | 7.066 | 5.679 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL A | 20144.831 | 6.559 | 6.564 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.232 | 5.988 | 7.845 | 1.00 | 0.00 C |
| ATOM | 236 | O | VAL A | 20143.373 | 6.610 | 8.471 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20145.845 | 7.660 | 6.930 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20147.003 | 7.079 | 7.729 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VALA | 20146.352 | 8.359 | 5.677 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.776 | 8.020 | 5.455 | 1.00 | 0.00 H |
| ATOM | 241 | НА | VAL A | 20145.358 | 5.773 | 6.043 | 1.00 | 0.00 H |
| ATOM | 242 | НВ | VAL A | 20145.345 | 8.392 | 7.547 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20147.813 | 7.792 | 7.760 | 1.00 | 0.00 H |

| ATOM | 244 2 | 2HG1 | VAL A | 20147.342 | 6.167 | 7.260 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 245 3 | BHG1 | VAL A | 20146.674 | 6.864 | 8.735 | 1.00 | 0.00 H |
| ATOM | 246 1 | HG2 | VAL A | 20146.407 | 9.423 | 5.856 | 1.00 | 0.00 H |
| ATOM | 247 2 | 2HG2 | VALA | 20145.676 | 8.167 | 4.858 | 1.00 | 0.00 H |
| ATOM | 248 3 | 3HG2 | VAL A | 20147.335 | 7.985 | 5.429 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.691 | 4.802 | 8.230 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.189 | 4.168 | 9.435 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.139 | 3.114 | 9.141 | 1.00 | 0.00 C |
| ATOM | 252 | O | GLY A | 21142.996 | 2.145 | 9.887 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.376 | 4.354 | 7.691 | 1.00 | 0.00 H |
| ATOM | 254 | lHA | GLY A | 21145.013 | 3.703 | 9.954 | 1.00 | 0.00 H |
| ATOM | 255 2 | 2HA | GLY A | 21143.756 | 4.923 | 10.072 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.400 | 3.304 | 8.051 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.358 | 2.363 | 7.661 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.934 | 1.233 | 6.815 | 1.00 | 0.00 C |
| ATOM | 259 | О | SER A | 22142.916 | 1.420 | 6.095 | 1.00 | 0.00 O |
| ATOM | 260 | СВ | SER A | 22140.255 | 3.084 | 6.886 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22139.291 | 3.639 | 7.764 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.561 | 4.097 | 7.498 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22140.936 | 1.943 | 8.563 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.690 | 3.882 | 6.302 | 1.00 | 0.00 H |
| ATOM | 265 | 2HB | SER A | 22139.763 | 2.384 | 6.227 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22139.736 | 4.075 | 8.494 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.319 | 0.059 | 6.906 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.771 | -1.103 | 6.149 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.219 | -1.074 | 4.727 | 1.00 | 0.00 C |
| ATOM | 270 | O | LEU A | 23140.087 | -0.646 | 4.499 | 1.00 | 0.00 O |

| ATOM | 271 | CB | LEU A | 23141.341 | -2.394 | 6.849 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 272 | CG | LEU A | 23142.012 | -2.651 | 8.199 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23141.094 | -3.458 | 9.106 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.339 | -3.369 | 8.005 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.542 | -0.029 | 7.497 | 1.00 | 0.00 H |
| ATOM | 276 | НА | LEU A | 23142.849 | -1.070 | 6.104 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.273 | -2.356 | 7.002 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.566 | -3.224 | 6.197 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.211 | -1.706 | 8.682 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23140.445 | -4.074 | 8.503 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23140.499 | -2.784 | 9.705 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23141.689 | -4.085 | 9.753 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23143.169 | -4.436 | 7.969 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23143.997 | -3.138 | 8.830 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23143.792 | -3.046 | 7.080 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.025 | -1.531 | 3.776 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.617 | -1.558 | 2.376 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALAA | 24142.162 | -2.794 | 1.669 | 1.00 | 0.00 C |
| ATOM | 289 | О | ALA A | 24143.002 | -3.511 | 2.211 | 1.00 | 0.00 O |
| ATOM | 290 | СВ | ALA A | 24142.082 | -0.294 | 1.668 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.916 | -1.859 | 4.019 | 1.00 | 0.00 H |
| ATOM | 292 | НА | ALA A | 24140.538 | -1.584 | 2.345 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALAA | 24143.093 | -0.432 | 1.314 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24142.051 | 0.537 | 2.357 | 1.00 | 0.00 H |
| ATOM | 295 | 3НВ | ALA A | 24141.432 | -0.091 | 0.830 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.678 | -3.036 | 0.456 | 1.00 | 0.00 N |
| ATOM | 297 | ' CA | GLU A | 25142.117 | -4.186 | -0.326 | 1.00 | 0.00 C |

| ATOM | 298 | C | GLU A | 25142.455 | -3.774 | -1.756 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 299 | О | GLU A | 25141.823 | -2.884 | -2.323 | 1.00 | 0.00 O |
| ATOM | 300 | СВ | GLU A | 25141.032 | -5.265 | -0.338 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.479 | -6.569 | -0.978 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.325 | -7.520 | -1.231 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25140.422 | -8.335 | -2.172 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25139.324 | -7.450 | -0.486 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25141.010 | -2.427 | 0.076 | 1.00 | 0.00 H |
| ATOM | 306 | HA | GLU A | 25143.004 | -4.585 | 0.140 | 1.00 | 0.00 H |
| ATOM | 307 | 1HB | GLU A | 25140.736 | -5.472 | 0.680 | 1.00 | 0.00 H |
| ATOM | 308 | 2HB | GLU A | 25140.178 | -4.896 | -0.885 | 1.00 | 0.00 H |
| ATOM | 309 | 1HG | GLU A | 25141.955 | -6.348 | -1.921 | 1.00 | 0.00 H |
| ATOM | 310 | 2HG | GLU A | 25142.188 | -7.053 | -0.323 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.459 | -4.429 | -2.333 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.882 | -4.131 | -3.695 | 1.00 | 0.00 C |
| ATOM | 313 | C | VAL A | 26143.519 | -5.267 | -4.644 | 1.00 | 0.00 C |
| ATOM | 314 | О | VAL A | 26143.657 | -6.442 | -4.305 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VALA | 26145.400 | -3.881 | -3.770 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VALA | 26145.791 | -3.373 | -5.149 | 1.00 | 0.00°C |
| ATOM | 317 | CG2 | VALA | 26145.833 | -2.901 | -2.690 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.925 | -5.129 | -1.829 | 1.00 | 0.00 H |
| ATOM | 319 | HA | VAL A | 26143.374 | -3.233 | -4.014 | 1.00 | 0.00 H |
| ATOM | 320 | HB | VAL A | 26145.908 | -4.819 | -3.600 | 1.00 | 0.00 H |
| ATOM | 321 | 1HG1 | VAL A | 26145.889 | -2.297 | -5.123 | 1.00 | 0.00 H |
| ATOM | 322 | 2HG1 | VAL A | 26145.030 | -3.648 | -5.864 | 1.00 | 0.00 H |
| ATOM | 323 | 3HG1 | VAL A | 26146.734 | -3.812 | -5.440 | 1.00 | 0.00 H |
| ATOM | 324 | 1HG2 | VAL A | 26145.367 | -3.169 | -1.753 | 1.00 | 0.00 H |

| ATOM | 325 2 | HG2 | VAL A | 26145.533 | -1.902 | -2.968 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 326 3 | HG2 | VAL A | 26146.907 | -2.938 | -2.582 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYSA | 27143.052 | -4.909 | -5.837 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27142.669 | -5.900 | -6.836 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27143.868 | -6.308 | -7.685 | 1.00 | 0.00 C |
| ATOM | 330 | О | LYS A | 27144.189 | -5.657 | -8.680 | 1.00 | 0.00 O |
| ATOM | 331 | СВ | LYS A | 27141.557 | -5.347 | -7.731 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.454 | -6.352 | -8.020 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYSA | 27139.652 | -6.674 | -6.770 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27138.931 | -5.445 | -6.239 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27139.738 | -4.727 | -5.213 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27142.964 | -3.957 | -6.049 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27142.299 | -6.770 | -6.315 | 1.00 | 0.00 H |
| ATOM | 338 1 | НВ | LYS A | 27141.115 | -4.489 | -7.248 | 1.00 | 0.00 H |
| ATOM | 339 2 | HB | LYS A | 27141.988 | -5.037 | -8.672 | 1.00 | 0.00 H |
| ATOM | 340 1 | HG | LYSA | 27139.790 | -5.939 | -8.765 | 1.00 | 0.00 H |
| ATOM | 341 2 | HG | LYSA | 27140.898 | -7.262 | -8.397 | 1.00 | 0.00 H |
| ATOM | 342 1 | HD | LYS A | 27138.922 | -7.433 | -7.007 | 1.00 | 0.00 H |
| ATOM | 343 2 | 2HD | LYS A | 27140.324 | -7.043 | -6.008 | 1.00 | 0.00 H |
| ATOM | 344 1 | HE | LYS A | 27138.735 | -4.775 | -7.063 | 1.00 | 0.00 H |
| ATOM | 345 2 | HE | LYS A | 27137.996 | -5.755 | -5.797 | 1.00 | 0.00 H |
| ATOM | 346 1 | HZ | LYS A | 27140.748 | -4.947 | -5.335 | 1.00 | 0.00 H |
| ATOM | 347 2 | 2HZ | LYS A | 27139.443 | -5.018 | -4.260 | 1.00 | 0.00 H |
| ATOM | 348 3 | BHZ | LYS A | 27139.603 | -3.701 | -5.308 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28144.529 | -7.390 | -7.286 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28145.694 | -7.886 | -8.010 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.709 | -9.411 | -8.036 | 1.00 | 0.00 C |

| ATOM | 352 | О | GLU A | 28144.797 | -10.059 | -7.525 | 1.00 | 0.00 O |
|------|-----|------|-------|-------------|-----------|--------|------|--------|
| ATOM | 353 | СВ | GLU A | 28146.980 | -7.360 | -7.368 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28147.981 | -6.812 | -8.372 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28149.350 | -6.580 | -7.762 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28149.538 | -5.534 | -7.106 | 1.00 | 0.00·O |
| ATOM | 357 | OE2 | GLU A | 28150.233 | -7.446 | -7.941 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.225 | -7.867 | -6.485 | 1.00 | 0.00 H |
| ATOM | 359 | HA | GLU A | 28145.633 | -7.520 | -9.024 | 1.00 | 0.00 H |
| ATOM | 360 | 1HB | GLU A | 28146.727 | -6.570 | -6.677 | 1.00 | 0.00 H |
| ATOM | 361 | 2HB | GLU A | 28147.453 | -8.164 | -6.824 | 1.00 | 0.00 H |
| ATOM | 362 | 1HG | GLU A | 28148.080 | -7.517 | -9.183 | 1.00 | 0.00 H |
| ATOM | 363 | 2HG | GLU A | 28147.609 | -5.873 | -8.755 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29146.752 | -9.977 | -8.635 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29146.886 | -11.426 | -8.726 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29146.958 | -12.052 | -7.335 | 1.00 | 0.00 C |
| ATOM | 367 | Ο | ASN A | 29146.123 | -12.880 | -6.974 | 1.00 | 0.00 O |
| ATOM | 368 | CB | ASN A | 29148.133 | -11.794 | -9.533 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29147.812 | -12.105 - | 10.982 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29147.758 | -13.268 - | 11.382 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29147.598 | -11.063 - | 11.777 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29147.448 | -9.407 | -9.023 | 1.00 | 0.00 H |
| ATOM | 373 | НА | ASN A | 29146.013 | -11.808 | -9.235 | 1.00 | 0.00 H |
| ATOM | 374 | 1HB | ASN A | 29148.828 | -10.969 | -9.507 | 1.00 | 0.00 H |
| ATOM | 375 | 2HB | ASN A | 29148.597 | -12.664 | -9.092 | 1.00 | 0.00 H |
| ATOM | 376 | 1HD2 | ASN A | 29147.658 - | 10.166 -1 | 1.389 | 1.00 | 0.00 H |
| ATOM | 377 | 2HD2 | ASN A | 29147.388 - | 11.235 -1 | 2.719 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30147.964 | -11.661 | -6.533 | 1.00 | 0.00 N |
| | | | | | | | | |

| ATOM | 379 | CA | PRO A | 30148.142 -12.186 | -5.177 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------------|--------|------|--------|
| ATOM | 380 | С | PRO A | 30147.167 -11.559 | -4.180 | 1.00 | 0.00 C |
| АТОМ | 381 | О | PRO A | 30147.291 -10.383 | -3.839 | 1.00 | 0.00 O |
| ATOM | 382 | СВ | PRO A | 30149.577 -11.785 | -4.840 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30149.809 -10.537 | -5.617 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30149.006 -10.676 | -6.885 | 1.00 | 0.00 C |
| ATOM | 385 | НА | PRO A | 30148.048 -13.261 | -5.151 | 1.00 | 0.00 H |
| ATOM | 386 1 | НВ | PRO A | 30149.666 -11.614 | -3.777 | 1.00 | 0.00 H |
| ATOM | 387 2 | НВ | PRO A | 30150.254 -12.571 | -5.143 | 1.00 | 0.00 H |
| ATOM | 388 1 | HG | PRO A | 30149.468 -9.684 | -5.050 | 1.00 | 0.00 H |
| ATOM | 389 2 | HG | PRO A | 30150.859 -10.438 | -5.849 | 1.00 | 0.00 H |
| ATOM | 390 1 | HD | PRO A | 30148.564 -9.730 | -7.156 | 1.00 | 0.00 H |
| ATOM | 391 2 | HD | PRO A | 30149.628 -11.045 | -7.685 | 1.00 | 0.00 H |
| ATOM | 392 | N | PRO A | 31146.181 -12.338 | -3.697 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31145.190 -11.843 | -2.736 | 1.00 | 0.00 C |
| ATOM | 394 | C | PRO A | 31145.794 -11.586 | -1.360 | 1.00 | 0.00 C |
| ATOM | 395 | O | PRO A | 31146.067 -12.521 | -0.606 | 1.00 | 0.00 O |
| ATOM | 396 | CB | PRO A | 31144.165 -12.976 | -2.667 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31144.925 -14.198 | -3.043 | 1.00 | 0.00 C |
| ATOM | 398 | CD | PRO A | 31145.955 -13.754 | -4.044 | 1.00 | 0.00 C |
| ATOM | 399 | HA | PRO A | 31144.712 -10.941 | -3.091 | 1.00 | 0.00 H |
| ATOM | 400 1 | НВ | PRO A | 31143.770 -13.047 | -1.663 | 1.00 | 0.00 H |
| ATOM | 401 2 | 2HB | PRO A | 31143.361 -12.782 | -3.362 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31145.408 -14.615 | -2.170 | 1.00 | 0.00 H |
| ATOM | 403 2 | HG | PRO A | 31144.260 -14.924 | -3.487 | 1.00 | 0.00 H |
| ATOM | 404 1 | HD | PRO A | 31146.863 -14.327 | -3.934 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31145.569 -13.846 | -5.048 | 1.00 | 0.00 H |

| ATOM | 406 | N | PHE A | 32146.001 | -10.313 | -1.038 | 1.00 | 0.00 N |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 407 | CA | PHE A | 32146.574 | -9.933 | 0.248 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.715 | -8.877 | 0.935 | 1.00 | 0.00 C |
| ATOM | 409 | O | PHE A | 32144.802 | -8.315 | 0.330 | 1.00 | 0.00 O |
| ATOM | 410 | СВ | PHE A | 32147.998 | -9.406 | 0.061 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.118 | -8.373 | -1.023 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.820 | -8.648 | -2.186 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32147.530 | -7.127 | -0.877 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.933 | -7.700 | -3.184 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.641 | -6.173 | -1.873 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.342 | -6.460 | -3.028 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.764 | -9.613 | -1.680 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.606 | -10.815 | 0.870 | 1.00 | 0.00 H |
| ATOM | 419 1 | НВ | PHE A | 32148.333 | -8.959 | 0.985 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.649 | -10.231 | -0.190 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32149.281 | -9.617 | -2.308 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32146.982 | -6.901 | 0.025 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32149.483 | -7.927 | -4.086 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32147.178 | -5.206 | -1.748 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.429 | -5.718 | -3.807 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.012 | -8.612 | 2.203 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.266 | -7.623 | 2.973 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.213 | -6.681 | 3.708 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.222 | -7.110 | 4.269 | 1.00 | 0.00 O |
| ATOM | 430 | СВ | TYR A | 33144.340 | -8.318 | 3.973 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.079 | -8.869 | 3.348 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.709 | -10.196 | 3.538 | 1.00 | 0.00 C |

| ATOM | 433 | CD2 | TYR A | 33142.257 | -8.064 | 2.568 | 1.00 | 0.00 C |
|------|-------|---------------------------|-------|-------------|---------|-------|------|--------|
| ATOM | 434 | CE1 | TYR A | 33141.557 - | 10.703 | 2.969 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.103 | -8.566 | 1.996 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.758 | -9.885 | 2.199 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.610 | -10.387 | 1.630 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.751 | -9.094 | 2.631 | 1.00 | 0.00 H |
| ATOM | 439 | HA | TYR A | 33144.669 | -7.047 | 2.282 | 1.00 | 0.00 H |
| ATOM | 440 1 | НВ | TYR A | 33144.869 | -9.139 | 4.432 | 1.00 | 0.00 H |
| ATOM | 441 2 | HB | TYR A | 33144.051 | -7.610 | 4.736 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33143.337 | -10.833 | 4.141 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.531 | -7.032 | 2.411 | 1.00 | 0.00 H |
| ATOM | 444 | ΉE1 | TYR A | 33141.286 - | 11.737 | 3.127 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.477 | -7.924 | 1.393 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.802 | -11.228 | 1.209 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.881 | -5.394 | 3.704 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.711 | -4.411 | 4.374 | 1.00 | 0.00 C |
| ATOM | 449 | $\mathbf{C}_{\mathbf{c}}$ | GLY A | 34145.948 | -3.149 | 4.725 | 1.00 | 0.00 C |
| ATOM | 450 | O | GLY A | 34144.896 | -2.873 | 4.150 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.066 | -5.109 | 3.241 | 1.00 | 0.00 H |
| ATOM | 452 1 | НА | GLY A | 34147.103 | -4.846 | 5.282 | 1.00 | 0.00 H |
| ATOM | 453 2 | HA | GLY A | 34147.537 | -4.151 | 3.727 | 1.00 | 0.00 H |
| ATOM | 454 | N . | VAL A | 35146.480 | -2.382 | 5.671 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VALA | 35145.842 | -1.143 | 6.098 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.536 | 0.070 | 5.486 | 1.00 | 0.00 C |
| ATOM | 457 | О | VAL A | 35147.743 | 0.052 | 5.247 | 1.00 | 0.00 C |
| ATOM | 458 | СВ | VAL A | 35145.848 | -1.009 | 7.635 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.273 | -0.996 | 8.169 | 1.00 | 0.00 C |

| ATOM | 460 | CG2 | VAL A | 35145.095 | 0.240 | 8.067 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 461 | Н | VAL A | 35147.322 | -2.656 | 6.092 | 1.00 | 0.00 H |
| ATOM | 462 | НА | VAL A | 35144.816 | -1.165 | 5.763 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.342 | -1.869 | 8.050 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VAL A | 35147.344 | -0.295 | 8.987 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35147.950 | -0.699 | 7.381 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VAL A | 35147.536 | -1.984 | 8.516 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VALA | 35145.576 | 1.113 | 7.652 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VAL A | 35145.096 | 0.307 | 9.145 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VAL A | 35144.076 | 0.188 | 7.712 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.764 | 1.122 | 5.233 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.305 | 2.343 | 4.648 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.257 | 3.039 | 5.615 | 1.00 | 0.00 C |
| ATOM | 473 | O | ILE A | 36147.061 | 3.001 | 6.830 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.182 | 3.324 | 4.253 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.129 | 2.611 | 3.400 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILE A | 36145.758 | 4.516 | 3.505 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.990 | 3.510 | 2.971 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.808 | 1.075 | 5.445 | 1.00 | 0.00 H |
| ATOM | 479 | HA | ILE A | 36146.848 | 2.073 | 3.754 | 1.00 | 0.00 H |
| ATOM | 480 | НВ | ILE A | 36144.717 | 3.687 | 5.157 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.599 | 2.224 | 2.509 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.711 | 1.791 | 3.967 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36146.253 | 5.174 | 4.204 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36144.960 | 5.051 | 3.011 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36146.469 | 4.172 | 2.770 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36142.253 | 3.558 | 3.759 | 1.00 | 0.00 H |

2.076 1.00 0.00 H487 2HD1 ILE A 36142.535 3.111 **ATOM** 4.500 2.772 1.00 0.00 H 488 3HD1 ILE A 36143.369 **ATOM** 5.067 1.00 0.00 N **ATOM** 489 N ARG A 37148.287 3.674 5.882 1.00 0.00 C 490 CA ARG A 37149.271 4.379 **ATOM** 0.00 C 491 C ARG A 37149.476 5.804 5.378 1.00 **ATOM** 0.00 O ARG A 37149.174 6.769 6.080 1.00 **ATOM** 492 Ο 0.00 C 493 ARG A 37150.604 3.626 5.872 1.00 CB**ATOM** 494 CG ARG A 37150.463 2.137 6.139 1.00 0.00 C **ATOM** ARG A 37149.863 0.00 C CD 1.870 7.511 1.00 495 **ATOM** NE ARG A 37150.865 1.945 8.571 1.00 0.00 N 496 **ATOM** 0.00 C 9.847 **ATOM** 497 CZ ARG A 37150.616 1.661 1.00 10.226 1.00 0.00 N NH1 ARG A 37149.401 1.284 **ATOM** 498 NH2 ARG A 37151.585 1.755 10.749 1.00 0.00 N **ATOM** 499 4.093 1.00 0.00 H ARG A 37148.389 3.668 **ATOM** 500 Η 6.893 1.00 0.00 H 501 HA ARGA 37148.897 4.418 **ATOM** 4.907 1.00 0.00 H **ATOM** 502 1HB ARG A 37151.069 3.754 1.00 0.00 H37151.247 6.632 **ATOM** 503 2HB ARG A 4.047 37149.820 1.705 5.386 1.00 0.00 H504 1HG ARGA **ATOM** 0.00 H 6.088 1.00 37151.440 1.678 **ATOM** 505 2HG ARGA 7.702 1.00 0.00 H 37149.095 2.605 506 1HD ARG A **ATOM** 7.511 1.00 0.00 H 507 2HD ARG A 37149.424 0.883 **ATOM** 1.00 0.00 H 508 HE ARGA 37151.770 2.221 8.319 **ATOM** 9.551 1.00 0.00 H **ATOM** 509 1HH1 ARG A 37148.667 1.211 11.187 1.00 0.00 H 37149.221 1.071 **ATOM** 510 2HH1 ARG A 511 1HH2 ARG A 37152.502 2.039 10.469 1.00 0.00 H **ATOM** 1.00 512 2HH2 ARG A 37151.398 11.707 0.00 H 1.542 **ATOM** 5.929 4.158 1.00 0.00 N TRPA 38149.989 **ATOM** 513 N

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| ATOM | 514 | CA | TRPA | 38150.233 | 7.238 | 3.563 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 515 | C | TRPA | 38149.491 | 7.382 | 2.237 | 1.00 | 0.00 C |
| ATOM | 516 | O | TRPA | 38149.514 | 6.481 | 1.399 | 1.00 | 0.00 O |
| ATOM | 517 | СВ | TRPA | 38151.735 | 7.456 | 3.349 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38152.054 | 8.673 | 2.533 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRP A | 38152.277 | 9.938 | 2.997 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRPA | 38152.180 | 8.741 | 1.107 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRPA | 38152.534 | 10.787 | 1.947 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.480 | 10.075 | 0.777 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38152.068 | 7.801 | 0.079 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRPA | 38152.669 | 10.492 | -0.540 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.256 | 8.216 | -1.226 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRPA | 38152.554 | 9.551 | -1.526 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRPA | 38150.208 | 5.122 | 3.646 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRPA | 38149.865 | 7.987 | 4.249 | 1.00 | 0.00 H |
| ATOM | 529 1 | HB | TRPA | 38152.215 | 7.565 | 4.310 | 1.00 | 0.00 H |
| ATOM | 530 2 | HB | TRP A | 38152.147 | 6.595 | 2.842 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38152.251 | 10.216 | 4.039 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38152.725 | 11.746 | 2.023 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRPA | 38151.838 | 6.769 | 0.289 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38152.896 | 11.518 | -0.788 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.173 | 7.503 | -2.034 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRPA | 38152.693 | 9.829 | -2.560 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.842 | 8.527 | 2.055 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39148.100 | 8.803 | 0.831 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILE A | 39148.544 | 10.127 | 0.223 | 1.00 | 0.00 C |
| ATOM | 540 | O | ILE A | 39148.213 | 11.197 | 0.735 | 1.00 | 0.00 O |

| ATOM | 541 | CB | ILE A | 39146.583 | 8.851 | 1.090 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 542 | CG1 | ILE A | 39146.137 | 7.619 | 1.880 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILEA | 39145.824 | 8.946 | -0.225 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.728 | 7.725 | 2.420 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.868 | 9.207 | 2.760 | 1.00 | 0.00 H |
| ATOM | 546 | HA | ILE A | 39148.302 | 8.007 | 0.129 | 1.00 | 0.00 H |
| ATOM | 547 | НВ | ILE A | 39146.366 | 9.737 | 1.667 | 1.00 | 0.00 H |
| ATOM | 548 | 1HG1 | ILE A | 39146.182 | 6.752 | 1.239 | 1.00 | 0.00 H |
| ATOM | 549 | 2HG1 | ILE A | 39146.804 | 7.476 | 2.717 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39146.045 | 8.080 | -0.832 | 1.00 | 0.00 H |
| ATOM | 551 | 2HG2 | ILE A | 39146.125 | 9.840 | -0.752 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39144.763 | 8.986 | -0.028 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.041 | 7.263 | 1.727 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39144.468 | 8.765 | 2.547 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39144.669 | 7.221 | 3.374 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.303 | 10.051 | -0.866 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.784 | 11.256 | -1.513 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.325 | 11.000 | -2.905 | 1.00 | 0.00 C |
| ATOM | 559 | Ο | GLY A | 40150.197 | 9.896 | -3.437 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.542 | 9.172 | -1.228 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40148.973 | 11.963 | -1.580 | 1.00 | 0.00 H |
| ATOM | 562 | 2HA | GLY A | 40150.569 | 11.684 | -0.909 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41150.931 | 12.024 | -3.494 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.497 | 11.918 | -4.833 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41152.964 | 12.346 | -4.832 | 1.00 | 0.00 C |
| ATOM | 566 | О | GLN A | 41153.276 | 13.509 | -4.574 | 1.00 | 0.00 O |
| ATOM | 567 | CB | GLN A | 41150.698 | 12.783 | -5.807 | 1.00 | 0.00 C |

0.00 C -5.716 1.00 **ATOM** 568 CG GLN A 41149.196 12.573 -5.845 1.00 0.00 C 13.867 **ATOM** 569 CD GLN A 41148.417 1.00 0.00O14.671 -4.914 **ATOM** 570 OE1 GLN A 41148.369 -7.002 1.00 0.00 N 14.074 **ATOM** 571 NE2 GLN A 41147.802 -3.016 1.00 0.00 H 41150.998 12.876 **ATOM** 572 H GLN A **ATOM** 573 HA GLN A 41151.430 10.886 -5.142 1.00 0.00 H1.00 -5.600 0.00 H41150.906 13.822 **ATOM** 574 1HB GLN A -6.814 1.00 0.00 H41151.013 12.556 **ATOM** 575 2HB GLN A 11.906 -6.508 1.00 0.00 H**ATOM** 576 1HG GLN A 41148.889 -4.761 1.00 0.00 H 41148.965 12.125 **ATOM** 577 2HG GLN A 578 1HE2 GLN A 41147.884 13.389 -7.698 1.00 0.00 H**ATOM** 1.00 579 2HE2 GLN A 41147.291 14.902 -7.114 0.00 H**ATOM** 1.00 0.00 N 11.412 -5.117 42153.889 **ATOM** 580 N PRO A 1.00 0.00 C CA PRO A 42155.326 11.708 -5.142 **ATOM** 581 1.00 0.00 C 42155.671 12.825 -6.122 C PRO A **ATOM** 582 42154.902 13.119 -7.038 1.00 0.00 O 583 O PRO A **ATOM** 42155.961 10.387 -5.590 1.00 0.00 C **ATOM** 584 CBPRO A -5.249 1.00 0.00 C 585 CG PRO A 42154.953 9.346 **ATOM** CD PRO A 42153.614 10.000 -5.435 1.00 0.00 C **ATOM** 586 42155.691 11.970 -4.1601.00 0.00 HPRO A **ATOM** 587 HA 42156.152 10.420 -6.653 1.00 0.00 H588 1HB PRO A **ATOM** 42156.886 10.230 -5.057 1.00 0.00 H **ATOM** 589 2HB PRO A 42155.054 8.501 -5.913 1.00 0.00 H 590 1HG PRO A **ATOM** 42155.078 9.034 -4.222 1.00 0.00 H **ATOM** 591 2HG PRO A 1.00 0.00 H 42153.280 9.891 -6.457**ATOM** 592 1HD PRO A 0.00 H42152.891 9.583 -4.7511.00 593 2HD PRO A **ATOM** 0.00 N 594 N PRO A 43156.841 13.463 -5.943 1.00 **ATOM**

| ATOM | 595 | CA | PRO A | 43157.286 | 14.551 | -6.816 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|----------|---------|------|--------|
| ATOM | 596 | C | PRO A | 43157.707 | 14.053 | -8.193 | 1.00 | 0.00 C |
| ATOM | 597 | O | PRO A | 43158.879 | 13.762 | -8.429 | 1.00 | 0.00 O |
| ATOM | 598 | CB | PRO A | 43158.488 | 15.132 | -6.072 | 1.00 | 0.00 C |
| ATOM | 599 | CG | PRO A | 43159.013 | 14.001 | -5.259 | 1.00 | 0.00 C |
| ATOM | 600 | CD | PRO A | 43157.817 | 13.173 | -4.876 | 1.00 | 0.00 C |
| ATOM | 601 | HA | PRO A | 43156.525 | 15.310 | -6.925 | 1.00 | 0.00 H |
| ATOM | 602 1 | НВ | PRO A | 43159.220 | 15.481 | -6.786 | 1.00 | 0.00 H |
| ATOM | 603 2 | 2HB | PRO A | 43158.167 | 15.952 | -5.447 | 1.00 | 0.00 H |
| ATOM | 604 1 | HG | PRO A | 43159.702 | 13.414 | -5.848 | 1.00 | 0.00 H |
| ATOM | 605 2 | 2HG | PRO A | 43159.504 | 14.381 | -4.375 | 1.00 | 0.00 H |
| ATOM | 606 1 | IHD | PRO A | 43158.074 | 12.124 | -4.864 | 1.00 | 0.00 H |
| ATOM | 607 2 | 2HD | PRO A | 43157.438 | 13.479 | -3.913 | 1.00 | 0.00 H |
| ATOM | 608 | N | GLY A | 44156.742 | 13.956 | -9.102 | 1.00 | 0.00 N |
| ATOM | 609 | CA | GLY A | 44157.035 | 13.493 - | -10.444 | 1.00 | 0.00 C |
| ATOM | 610 | C | GLY A | 44155.815 | 12.935 - | 11.146 | 1.00 | 0.00 C |
| ATOM | 611 | O | GLY A | 44155.511 | 13.319 - | 12.275 | 1.00 | 0.00 O |
| ATOM | 612 | Н | GLY A | 44155.826 | 14.202 | -8.859 | 1.00 | 0.00 H |
| ATOM | 613 | lHA | GLY A | 44157.422 | 14.318 - | 11.021 | 1.00 | 0.00 H |
| ATOM | 6142 | 2HA | GLY A | 44157.789 | 12.721 - | 10.389 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45155.112 | 12.028 - | 10.476 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEU A | 45153.916 | 11.419 | -11.047 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45152.704 | 11.673 - | 10.162 | 1.00 | 0.00 C |
| ATOM | 618 | O | LEU A | 45152.622 | 11.161 | -9.045 | 1.00 | 0.00 O |
| ATOM | 619 | CB | LEU A | 45154.123 | 9.914 | -11.228 | 1.00 | 0.00 C |
| ATOM | 620 | CG | LEU A | 45154.702 | 9.190 | -10.012 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.398 | 7.699 - | 10.079 | 1.00 | 0.00 C |

622 CD2 LEU A 45156.202 9.431 -9.913 1.00 0.00 C **ATOM** LEU A 45155.402 1.00 0.00 H **ATOM** 623 Η 11.763 -9.577 HA LEUA 45153.744 11.868 -12.013 1.00 0.00 H **ATOM** 624 LEU A 45153.168 9.467 -11.467 1.00 0.00 H **ATOM** 625 1HB **ATOM** 626 2HB LEU A 45154.792 9.761 -12.061 1.00 0.00 H 9.583 -9.116 1.00 0.00 H **ATOM** 627 HG LEUA 45154.240 7.394 -9.174 1.00 0.00 H **ATOM** 628 1HD1 LEU A 45153.895 **ATOM** 629 2HD1 LEU A 45155.321 7.147 -10.182 1.00 0.00 H630 3HD1 LEU A 45153.763 7.498 -10.930 1.00 **ATOM** 0.00 H10.107 -9.095 1.00 **ATOM** 631 1HD2 LEU A 45156.405 0.00 H**ATOM** 632 2HD2 LEU A 45156.558 9.867 -10.836 1.00 0.00 H8.493 -9.739 1.00 0.00 H**ATOM** 633 3HD2 LEU A 45156.709 12.464 -10.662 1.00 0.00 N **ATOM** 634 N ASN A 46151.760 12.771 -9.903 1.00 0.00 C **ATOM** 635 CA ASNA 46150.556 ASN A 636 \mathbf{C} 46149.628 11.563 -9.860 1.00 0.00 C **ATOM ATOM** 637 0 ASN A 46149.007 11.207 -10.861 1.00 0.00 O 46149.829 **ATOM** 638 CB ASN A 13.967 -10.521 1.00 0.00 C 46148.973 14.709 -9.514 1.00 0.00 C **ATOM** 639 CG ASN A OD1 ASN A **ATOM** 640 46147.746 14.622 -9.540 1.00 0.00 O 46149.619 15.445 -8.617 1.00 0.00 N **ATOM** 641 ND2 ASN A 642 Η ASN A 46151.875 12.844 -11.558 1.00 0.00 H**ATOM** HA ASN A 46150.852 13.021 -8.895 1.00 0.00 H **ATOM** 643 644 1HB ASN A 46150.557 14.655 -10.922 1.00 0.00 H**ATOM** 645 2HB ASN A 46149.191 13.619 -11.320 1.00 0.00 H**ATOM** 646 1HD2 ASN A 46150.599 15.468 -8.655 1.00 0.00 H**ATOM** 647 2HD2 ASN A 46149.091 15.936 -7.953 1.00 0.00 H**ATOM ATOM** 648 N GLUA 47149.543 10.935 -8.693 1.00 0.00 N

| ATOM | 649 | CA | GLU A | 47148.693 | 9.766 | -8.511 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|---------|---------|------|--------|
| ATOM | 650 | C | GLU A | 47148.523 | 9.444 | -7.031 | 1.00 | 0.00 C |
| ATOM | 651 | O | GLU A | 47149.502 | 9.193 | -6.327 | 1.00 | 0.00 O |
| ATOM | 652 | CB | GLU A | 47149.286 | 8.558 | -9.243 | 1.00 | 0.00 C |
| ATOM | 653 | CG | GLU A | 47150.801 | 8.468 | -9.150 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.389 | 7.499 | -10.156 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.498 | 7.871 - | 11.345 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.742 | 6.370 | -9.757 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47150.064 | 11.268 | -7.933 | 1.00 | 0.00 H |
| ATOM | 658 | HA | GLU A | 47147.725 | 9.991 | -8.932 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.866 | 7.656 | -8.820 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47149.014 | 8.615 - | -10.286 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47151.218 | 9.446 | -9.329 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47151.070 | 8.140 | -8.157 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.281 | 9.445 | -6.564 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VALA | 48146.998 | 9.146 | -5.167 | 1.00 | 0.00 C |
| ATOM | 665 | C | VAL A | 48147.382 | 7.708 | -4.839 | 1.00 | 0.00 C |
| ATOM | 666 | Ο | VAL A | 48146.654 | 6.771 | -5.164 | 1.00 | 0.00 O |
| ATOM | 667 | CB | VAL A | 48145.510 | 9.358 | -4.832 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VALA | 48145.280 | 9.261 | -3.332 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VAL A | 48145.028 | 10.698 | -5.367 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.539 | 9.647 | -7.171 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.586 | 9.814 | -4.555 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48144.938 | 8.577 | -5.311 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48146.009 | 9.870 | -2.816 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VAL A | 48145.384 | 8.234 | -3.018 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48144.286 | 9.612 | -3.096 | 1.00 | 0.00 H |

-6.435 1.00 $0.00 \, \text{H}^{-1}$ **ATOM** 676 1HG2 VAL A 48144.888 10.631 1.00 0.00 H 48145.764 11.458 -5.149 **ATOM** 677 2HG2 VAL A 48144.092 10.958 -4.896 1.00 0.00 H**ATOM** 678 3HG2 VAL A 7.539 -4.201 1.00 0.00 N 49148.535 **ATOM** 679 N LEU A 6.214 -3.836 1.00 0.00 C LEU A 49149.018 **ATOM** 680 CA **ATOM** 681 \mathbf{C} LEU A 49148.878 5.981 -2.338 1.00 0.00 C 1.00 6.638 -1.5320.00 O682 0 49149.538 **ATOM** LEU A 49150.480 6.046 -4.256 1.00 0.00 C CB LEU A **ATOM** 683 1.00 0.00 C 49150.733 6.129 -5.763**ATOM** 684 CG LEU A 1.00 0.00 C 49152.125 6.676 -6.041 685 CD1 LEU A **ATOM** CD2 LEU A 49150.556 4.763 -6.408 1.00 0.00 C **ATOM** 686 1.00 0.00 H687 LEU A 49149.075 8.325 -3.971**ATOM** Η 1.00 0.00 H49148.417 5.486 -4.360 **ATOM** 688 HA LEU A 1.00 0.00 H**ATOM** 689 1HB LEU A 49151.062 6.815 -3.771 5.084 -3.910 1.00 0.00 H690 2HB LEU A 49150.824 **ATOM** 691 HG LEUA 49150.016 6.805 -6.206 1.00 0.00 H**ATOM** -5.535 692 1HD1 LEU A 49152.859 6.065 1.00 0.00 H **ATOM** 7.691 -5.679 1.00 0.00 H**ATOM** 693 2HD1 LEU A 49152.192 694 3HD1 LEU A 49152.313 6.658 -7.104 1.00 0.00 H**ATOM** 0.00 H 49151.466 4.192 -6.2991.00 695 1HD2 LEU A **ATOM** 4.887 -7.458 1.00 0.00 H **ATOM** 696 2HD2 LEU A 49150.332 0.00 H 49149.744 4.241 -5.927 1.00 **ATOM** 697 3HD2 LEU A 50148.016 5.041 -1.969 1.00 0.00 N **ATOM** 698 N ALA A 50147.792 4.725 -0.5671.00 0.00 C **ATOM** 699 CA ALA A -0.1061.00 0.00 C \mathbf{C} **ALAA** 50148.710 3.597 **ATOM** 700 ALA A -0.5771.00 0.00 O 50148.601 2.465 **ATOM** 701 O -0.335 1.00 0.00 C **ATOM** 702 CB **ALAA** 50146.334 4.353

| ATOM | 703 | Н | ALA A | 50147.518 | 4.551 | -2.657 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 704 | НА | ALA A | 50148.009 | 5.613 | 0.009 | 1.00 | 0.00 H |
| ATOM | 705 | 1HB | ALA A | 50145.791 | 5.222 | 0.005 | 1.00 | 0.00 H |
| ATOM | 706 | 2HB | ALA A | 50146.275 | 3.576 | 0.412 | 1.00 | 0.00 H |
| ATOM | 707 | знв | ALA A | 50145.903 | 3.997 | -1.259 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.612 | 3.914 | 0.815 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.535 | 2.916 | 1.323 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51149.844 | 1.863 | 2.167 | 1.00 | 0.00 C |
| ATOM | 711 | О | GLY A | 51149.329 | 2.161 | 3.245 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.653 | 4.833 | 1.153 | 1.00 | 0.00 H |
| ATOM | 713 | 1HA | GLY A | 51151.018 | 2.431 | 0.488 | 1.00 | 0.00 H |
| ATOM | 714 | 2HA | GLY A | 51151.286 | 3.408 | 1.924 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.831 | 0.629 | 1.676 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.197 | -0.472 | 2.394 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.243 | -1.373 | 3.043 | 1.00 | 0.00 C |
| ATOM | 718 | О | LEU A | 52151.202 | -1.795 | 2.395 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.321 | -1.291 | 1.444 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.056 | -0.582 | 0.958 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.413 | -1.358 | -0.180 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52146.072 | -0.402 | 2.105 | 1.00 | 0.00 C |
| ATOM | 723 | H | LEU A | 52150.258 | 0.452 | 0.813 | 1.00 | 0.00 H |
| ATOM | 724 | HA | LEU A | 52148.576 | -0.048 | 3.168 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.914 | -1.558 | 0.582 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52148.025 | -2.197 | 1.951 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.320 | 0.398 | 0.587 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52147.183 | -1.760 | -0.823 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52145.776 | -0.698 | -0.752 | 1.00 | 0.00 H |

| ATOM | 730 | 3HD1 | LEU A | 52145.822 | -2.167 | 0.223 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 731 | 1HD2 | LEU A | 52146.235 | -1.174 | 2.843 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52145.063 | -0.473 | 1.728 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52146.220 | 0.567 | 2.558 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53150.052 | -1.664 | 4.326 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.978 | -2.514 | 5.063 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.455 | -3.945 | 5.146 | 1.00 | 0.00 C |
| ATOM | 737 | O | GLU A | 53149.489 | -4.223 | 5.858 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.204 | -1.959 | 6.470 | 1.00 | 0.00 C |
| ATOM | 739 | CG | GLU A | 53152.193 | -2.769 | 7.292 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.825 | -2.820 | 8.762 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53150.789 | -3.436 | 9.095 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53152.571 | -2.244 | 9.581 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53149.269 | -1.297 | 4.787 | 1.00 | 0.00 H |
| ATOM | 744 | HA | GLU A | 53151.919 | -2.519 | 4.532 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.577 | -0.949 | 6.391 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53150.259 | -1.944 | 6.995 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53152.219 | -3.779 | 6.909 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53153.172 | -2.323 | 7.196 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54151.097 | -4.848 | 4.413 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.696 | -6.250 | 4.404 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54150.964 | -6.903 | 5.757 | 1.00 | 0.00 C |
| ATOM | 752 | О | LEU A | 54152.037 | -6.735 | 6.335 | 1.00 | 0.00 O |
| ATOM | 753 | CB | LEU A | 54151.439 | -7.008 | 3.302 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.377 | -6.362 | 1.917 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.577 | -6.778 | 1.080 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54150.080 | -6.734 | 1.215 | 1.00 | 0.00 C |

| ATOM | 757 | Н | LEU A | 54151.859 | -4.565 | 3.866 | 1.00 | 0.00 H |
|------|-----|------|---------|-------------|---------|-------|------|--------|
| ATOM | 758 | HA | LEU A | 54149.635 | -6.290 | 4.203 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.476 | -7.094 | 3.591 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54151.019 | -8.000 | 3.231 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.404 | -5.288 | 2.026 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54152.294 | -6.815 | 0.038 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54152.914 | -7.755 | 1.396 | 1.00 | 0.00 H |
| ATOM | 764 | 3HD1 | LEU A | 54153.373 | - 6.062 | 1.212 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54150.087 | -6.336 | 0.212 | 1.00 | 0.00 H |
| ATOM | 766 | 2HD2 | LEU A | 54149.244 | -6.321 | 1.761 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.988 | -7.809 | 1.175 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55149.981 | -7.645 | 6.255 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55150.112 | -8.323 | 7.540 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55151.134 | -9.452 | 7.459 | 1.00 | 0.00 C |
| ATOM | 771 | Ο | GLU A | 55151.849 | -9.725 | 8.422 | 1.00 | 0.00 O |
| ATOM | 772 | CB | GLU A | 55148.758 | -8.876 | 7.988 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55147.661 | -7.825 | 8.049 | 1.00 | 0.00 C |
| ATOM | 774 | ČD | GLU A | 55146.606 | -8.144 | 9.089 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55146.111 | -7.202 | 9.743 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | 2 GLU A | 55146.273 | -9.338 | 9.250 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.149 | -7.740 | 5.746 | 1.00 | 0.00 H |
| ATOM | 778 | HA | GLU A | 55150.452 | -7.597 | 8.264 | 1.00 | 0.00 H |
| ATOM | 779 | 1HB | GLU A | 55148.450 | -9.646 | 7.297 | 1.00 | 0.00 H |
| ATOM | 780 | 2HB | GLU A | 55148.867 | -9.310 | 8.971 | 1.00 | 0.00 H |
| ATOM | 781 | 1HG | GLU A | 55148.106 | -6.873 | 8.292 | 1.00 | 0.00 H |
| ATOM | 782 | 2HG | GLU A | 55147.185 | -7.764 | 7.081 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56151.196 - | -10.104 | 6.302 | 1.00 | 0.00 N |

| ATOM | 784 | CA | ASPA | 56152.131 | -11.204 | 6.095 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 785 | C | ASPA | 56153.441 | -10.699 | 5.500 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASP A | 56153.443 | -9.875 | 4.585 | 1.00 | O.00 O |
| ATOM | 787 | CB | ASPA | 56151.513 | -12.260 | 5.178 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56151.896 | -13.671 | 5.579 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASPA | 56152.482 - | 14.388 | 4.741 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56151.612 | 14.057 | 6.733 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.601 | -9.839 | 5.571 | 1.00 | 0.00 H |
| ATOM | 792 | HA | ASPA | 56152.336 | -11.650 | 7.057 | 1.00 | 0.00 H |
| ATOM | 793 1 | НВ | ASPA | 56150.437 - | 12.175 | 5.214 | 1.00 | 0.00 H |
| ATOM | 794 2 | HB | ASPA | 56151.849 | 12.090 | 4.165 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.555 | -11.200 | 6.023 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57155.873 | -10.799 | 5.543 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.191 | -11.467 | 4.209 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57156.569 | -12.637 | 4.163 | 1.00 | 0.00 O |
| ATOM | 799 | CB | GLU A | 57156.945 | -11.158 | 6.573 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.202 | -10.058 | 7.591 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57158.675 | -9.895 | 7.913 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57159.507 | -10.090 | 7.002 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57158.996 | -9.573 | 9.076 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.490 | -11.854 | 6.750 | 1.00 | 0.00 H |
| ATOM | 805 | HA | GLU A | 57155.864 | -9.729 | 5.403 | 1.00 | 0.00 H |
| ATOM | 806 1 | HB | GLU A | 57156.635 | -12.045 | 7.106 | 1.00 | 0.00 H |
| ATOM | 807 2 | HB | GLU A | 57157.871 | -11.364 | 6.057 | 1.00 | 0.00 H |
| ATOM | 808 1 | HG | GLU A | 57156.832 | -9.125 | 7.194 | 1.00 | 0.00 H |
| ATOM | 809 2 | HG | GLU A | 57156.673 | -10.298 | 8.502 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58156.035 | -10.715 | 3.125 | 1.00 | 0.00 N |

| ATOM | 811 | CA | CYS A | 58156.305 - | 11.234 | 1.789 | 1.00 | 0.00 C | |
|------|-------|-----|-------|-------------|---------|--------|------|--------|---|
| ATOM | 812 | C | CYS A | 58157.612 - | 10.668 | 1.241 | 1.00 | 0.00 C | |
| ATOM | 813 | О | CYS A | 58157.877 | -9.472 | 1.350 | 1.00 | 0.00 O | |
| ATOM | 814 | СВ | CYS A | 58155.153 - | 10.892 | 0.844 | 1.00 | 0.00 C | |
| ATOM | 815 | SG | CYS A | 58154.828 - | 12.155 | -0.409 | 1.00 | 0.00 S | |
| ATOM | 816 | Н | CYS A | 58155.731 | -9.788 | 3.225 | 1.00 | 0.00 H | |
| ATOM | 817 | НА | CYS A | 58156.393 - | 12.307 | 1.862 | 1.00 | 0.00 H | |
| ATOM | 818 1 | НВ | CYS A | 58154.249 - | 10.764 | 1.421 | 1.00 | 0.00 H | |
| ATOM | 819 2 | 2HB | CYS A | 58155.378 | -9.970 | 0.330 | 1.00 | 0.00 H | |
| ATOM | 820 | HG | CYS A | 58155.382 | -11.967 | -1.171 | 1.00 | 0.00 H | • |
| ATOM | 821 | N | ALA A | 59158.424 - | 11.538 | 0.649 | 1.00 | 0.00 N | |
| ATOM | 822 | CA | ALAA | 59159.704 - | -11.127 | 0.083 | 1.00 | 0.00 C | |
| ATOM | 823 | C | ALA A | 59159.504 - | 10.336 | -1.206 | 1.00 | 0.00 C | |
| ATOM | 824 | О | ALA A | 59158.946 - | 10.845 | -2.177 | 1.00 | 0.00 O | |
| ATOM | 825 | СВ | ALA A | 59160.583 - | -12.342 | -0.172 | 1.00 | 0.00 C | |
| ATOM | 826 | H′ | ALA A | 59158.157 - | 12.480 | 0.592 | 1.00 | 0.00 H | |
| ATOM | 827 | HA | ALA A | 59160.201 | -10.498 | 0.806 | 1.00 | 0.00 H | |
| ATOM | 828 | lНВ | ALA A | 59160.533 - | 13.006 | 0.679 | 1.00 | 0.00 H | |
| ATOM | 829 2 | 2HB | ALA A | 59161.604 - | 12.022 | -0.319 | 1.00 | 0.00 H | |
| ATOM | 830 3 | ВНВ | ALA A | 59160.235 - | 12.859 | -1.053 | 1.00 | 0.00 H | |
| ATOM | 831 | N | GLY A | 60159.964 | -9.090 | -1.206 | 1.00 | 0.00 N | |
| ATOM | 832 | CA | GLY A | 60159.828 | -8.249 | -2.381 | 1.00 | 0.00 C | |
| ATOM | 833 | C | GLY A | 60159.332 | -6.857 | -2.044 | 1.00 | 0.00 C | |
| ATOM | 834 | O | GLY A | 60159.634 | -5.895 | -2.751 | 1.00 | 0.00 O | |
| ATOM | 835 | Н | GLY A | 60160.402 | -8.738 | -0.403 | 1.00 | 0.00 H | |
| ATOM | 836 | 1HA | GLY A | 60160.789 | -8.169 | -2.868 | 1.00 | 0.00 H | |
| ATOM | 837 | 2HA | GLY A | 60159.129 | -8.713 | -3.063 | 1.00 | 0.00 H | |

| ATOM | 838 | N | CYS A | 61158.569 | -6.749 | -0.961 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 839 | CA | CYS A | 61158.030 | -5.464 | -0.533 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.088 | -4.647 | 0.201 | 1.00 | 0.00 C |
| ATOM | 841 | О | CYS A | 61160.199 | -5.122 | 0.439 | 1.00 | 0.00 O |
| ATOM | 842 | CB | CYS A | 61156.814 | -5.674 | 0.372 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYS A | 61155.538 | -6.739 | -0.343 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.363 | -7.552 | -0.440 | 1.00 | 0.00 H |
| ATOM | 845 | HA | CYS A | 61157.721 | -4.923 | -1.414 | 1.00 | 0.00 H |
| ATOM | 846 | lНВ | CYS A | 61157.137 | -6.126 | 1.297 | 1.00 | 0.00 H |
| ATOM | 847 2 | 2HB | CYS A | 61156.361 | -4.716 | 0.584 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61155.374 | -6.443 | -1.241 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.736 | -3.416 | 0.557 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.656 | -2.532 | 1.265 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.205 | -2.320 | 2.707 | 1.00 | 0.00 C |
| ATOM | 852 | О | THR A | 62158.208 | -2.893 | 3.147 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62159.755 | -1.186 | 0.546 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.468 | -0.633 | 0.336 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.441 | -1.276 | -0.800 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62157.835 | -3.094 | 0.341 | 1.00 | 0.00 H |
| ATOM | 857 | HA | THR A | 62160.628 | -3.001 | 1.270 | 1.00 | 0.00 H |
| ATOM | 858 | HB | THR A | 62160.322 | -0.502 | 1.161 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62158.158 | -0.226 | 1.149 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62160.407 | -2.296 | -1.154 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62161.470 | -0.963 | -0.701 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62159.936 | -0.634 | -1.506 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63159.946 | -1.492 | 3.437 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASPA | 63159.622 | -1.204 | 4.830 | 1.00 | 0.00 C |

| ATOM | 865 | C | ASP A | 63158.872 | 0.118 | 4.951 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 866 | O | ASP A | 63158.994 | 0.823 | 5.953 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASP A | 63160.897 | -1.160 | 5.673 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.958 | -0.260 | 5.071 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63161.917 | 0.962 | 5.329 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63162.830 | -0.775 | 4.341 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASPA | 63160.728 | -1.066 | 3.030 | 1.00 | 0.00 H |
| ATOM | 872 | НА | ASPA | 63158.988 | -1.998 | 5.194 | 1.00 | 0.00 H |
| ATOM | 873 | lНВ | ASPA | 63160.658 | -0.792 | 6.659 | 1.00 | 0.00 H |
| ATOM | 874 2 | 2HB | ASP A | 63161.302 | -2.158 | 5.755 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64158.097 | 0.449 | 3.923 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.338 | 1.687 | 3.936 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64158.086 | 2.832 | 3.282 | 1.00 | 0.00 C |
| ATOM | 878 | О | GLY A | 64158.057 | 3.960 | 3.772 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64158.038 | -0.151 | 3.152 | 1.00 | 0.00 H |
| ATOM | 880 | 1HA | GLY A | 64156.408 | 1.532 | 3.409 | 1.00 | 0.00 H |
| ATOM | 881 2 | 2HA | GLY A | 64157.119 | 1.951 | 4.959 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.759 | 2.540 | 2.173 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.518 | 3.555 | 1.451 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65159.186 | 3.527 | -0.037 | 1.00 | 0.00 C |
| ATOM | 885 | О | THR A | 65159.401 | 2.520 | -0.712 | 1.00 | 0.00 O |
| ATOM | 886 | CB | THR A | 65161.018 | 3.339 | 1.654 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.361 | 1.979 | 1.450 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.498 | 3.730 | 3.036 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.743 | 1.622 | 1.832 | 1.00 | 0.00 H |
| ATOM | 890 | HA | THR A | 65159.246 | 4.520 | 1.851 | 1.00 | 0.00 H |
| ATOM | 891 | HB | THR A | 65161.559 | 3.937 | 0.935 | 1.00 | 0.00 H |

| ATOM | 892 | HG1 | THR A | 65160.987 | 1.675 | 0.620 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 893 | 1HG2 | THR A | 65161.971 | 2.882 | 3.507 | 1.00 | 0.00 H |
| ATOM | 894 | 2HG2 | THR A | 65160.656 | 4.050 | 3.632 | 1.00 | 0.00 H |
| ATOM | 895 | 3HG2 | THR A | 65162.209 | 4.539 | 2.954 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.661 | 4.639 | -0.541 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.299 | 4.742 | -1.950 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.221 | 5.716 | -2.679 | 1.00 | 0.00 C |
| ATOM | 899 | Ο | PHE A | 66159.301 | 6.892 | -2.326 | 1.00 | 0.00 O |
| ATOM | 900 | CB | PHE A | 66156.845 | 5.196 | -2.093 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.255 | 4.906 | -3.443 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.891 | 3.615 | -3.791 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66156.065 | 5.924 | -4.364 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.348 | 3.345 | -5.033 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.523 | 5.659 | -5.607 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66155.163 | 4.368 | -5.943 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.514 | 5.408 | 0.047 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66158.406 | 3.764 | -2.393 | 1.00 | 0.00 H |
| ATOM | 909 | 1HB | PHE A | 66156.243 | 4.691 | -1.353 | 1.00 | 0.00 H |
| ATOM | 910 | 2HB | PHE A | 66156.791 | 6.263 | -1.927 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66156.035 | 2.814 | -3.082 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.345 | 6.933 | -4.104 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66155.069 | 2.333 | -5.293 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.379 | 6.461 | -6.316 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.739 | 4.159 | -6.913 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.915 | 5.216 | -3.697 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67160.832 | 6.041 | -4.475 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.929 | 6.620 | -3.587 | 1.00 | 0.00 C |

| ATOM | 919 | О | ARG A | 67162.433 | 7.715 | -3.841 | 1.00 | 0.00 O |
|------|-------|------|-------|-----------|---------|--------|-------|--------|
| ATOM | 920 | СВ | ARG A | 67160.070 | 7.173 | -5.166 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67158.877 | 6.694 | -5.979 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67159.187 | 6.672 | -7.467 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67158.148 | 5.989 | -8.234 | ,1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67158.009 | 6.095 | -9.553 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67158.840 | 6.854 - | 10.257 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67157.035 | 5.440 - | 10.172 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.809 | 4.270 | -3.929 | 1.00 | 0.00 H |
| ATOM | 928 | НА | ARG A | 67161.287 | 5.413 | -5.225 | 1.00 | 0.00 H |
| ATOM | 929 | 1HB | ARG A | 67159.713 | 7.862 | -4.417 | 1.00 | 0.00 H |
| ATOM | 930 2 | 2HB | ARG A | 67160.746 | 7.692 | -5.830 | 1.00 | 0.00 H |
| ATOM | 931 | 1HG | ARG A | 67158.615 | 5.696 | -5.662 | 1.00 | 0.00 H |
| ATOM | 932 | 2HG | ARG A | 67158.045 | 7.361 | -5.805 | 1.00 | 0.00 H |
| ATOM | 933 | 1HD | ARG A | 67159.272 | 7.689 | -7.821 | 1.00 | 0.00 H |
| ATOM | 934 | 2HD | ARG A | 67160.127 | 6.161 | -7.618 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67157.520 | 5.422 | -7.739 | 1.00 | 0.00 H |
| ATOM | 936 | 1HH1 | ARG A | 67159.576 | 7.350 | -9.797 | 1.00 | 0.00 H |
| ATOM | 937 | 2HH1 | ARG A | 67158.731 | 6.929 - | 11.248 | 1.00 | 0.00 H |
| ATOM | 938 | 1HH2 | ARG A | 67156.407 | 4.867 | -9.647 | 1.00 | 0.00 H |
| ATOM | 939 | 2HH2 | ARG A | 67156.931 | 5.520 - | 11.163 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.294 | 5.880 | -2.546 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.328 | 6.336 | -1.637 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.851 | 7.452 | -0.728 | 1.00 | 0.00 C |
| ATOM | 943 | О | GLY A | 68163.645 | 8.277 | -0.277 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68161.858 | 5.016 | -2.394 | 1.00 | 0.00 H |
| ATOM | 945 | 1HA | GLY A | 68163.650 | 5.504 | -1.028 | 1.00 | 0.00 H |

| ATOM | 946 | 2HA | GLY A | 68164.169 | 6.692 | -2.215 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 947 | N | THR A | 69161.549 | 7.477 | -0.459 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.967 | 8.500 | 0.402 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69160.013 | 7.879 | 1.417 | 1.00 | 0.00 C |
| ATOM | 950 | O | THR A | 69158.835 | 7.665 | 1.126 | 1.00 | 0.00 O |
| ATOM | 951 | СВ | THR A | 69160.228 | 9.543 | -0.438 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69161.060 | 10.033 | -1.474 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69159.750 | 10.732 | 0.367 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.967 | 6.792 | -0.848 | 1.00 | 0.00 H |
| ATOM | 955 | HA | THR A | 69161.772 | 8.984 | 0.934 | 1.00 | 0.00 H |
| ATOM | 956 | НВ | THR A | 69159.362 | 9.079 | -0.889 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.864 | 10.397 | -1.095 | 1.00 | 0.00 H |
| ATOM | 958 | 1HG2 | THR A | 69158.755 | 11.006 | 0.048 | 1.00 | 0.00 H |
| ATOM | 959 | 2HG2 | THR A | 69160.421 | 11.564 | 0.214 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69159.732 | 10.473 | 1.416 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.528 | 7.590 | 2.608 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.721 | 6.993 | 3.665 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.604 | 7.938 | 4.097 | 1.00 | 0.00 C |
| ATOM | 964 | О | ARG A | 70158.855 | 9.085 | 4.463 | 1.00 | 0.00 O |
| ATOM | 965 | СВ | ARG A | 70160.598 | 6.640 | 4.867 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70159.836 | 5.977 | 6.004 | 1.00 | 0.00 C |
| ATOM | 967 | CD | ARG A | 70160.300 | 6.481 | 7.361 | 1.00 | 0.00 C |
| ATOM | 968 | NE | ARG A | 70160.874 | 5.412 | 8.175 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70161.488 | 5.614 | 9.338 | 1.00 | 0.00 C |
| ATOM | 970 | NH1 | ARG A | 70161.607 | 6.842 | 9.829 | 1.00 | 0.00 N |
| ATOM | 971 | NH2 | ARG A | 70161.982 | 4.586 | 10.014 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.472 | 7.783 | 2.779 | 1.00 | 0.00 H |
| | | | | | | | | |

| ATOM | 973 | НА | ARG A | 70159.279 | 6.088 | 3.274 | 1.00 | 0.00 H |
|--------|-----|----------|-------|-----------|--------|--------|------|--------|
| ATOM | 974 | 1HB | ARG A | 70161.378 | 5.965 | 4.544 | 1.00 | 0.00 H |
| ATOM | 975 | 2HB | ARG A | 70161.052 | 7.544 | 5.245 | 1.00 | 0.00 H |
| ATOM | 976 | 1HG | ARG A | 70158.784 | 6.193 | 5.892 | 1.00 | 0.00 H |
| ATOM | 977 | 2HG | ARG A | 70159.992 | 4.908 | 5.953 | 1.00 | 0.00 H |
| ATOM | 978 | 1HD | ARG A | 70161.046 | 7.247 | 7.213 | 1.00 | 0.00 H |
| ATOM | 979 | 2HD | ARG A | 70159.453 | 6.901 | 7.883 | 1.00 | 0.00 H |
| ATOM | 980 | HE | ARG A | 70160.800 | 4.496 | 7.836 | 1.00 | 0.00 H |
| ATOM | 981 | 1HH1 | ARG A | 70161.237 | 7.621 | 9.325 | 1.00 | 0.00 H |
| ATOM | 982 | 2HH1 | ARG A | 70162.069 | 6.987 | 10.705 | 1.00 | 0.00 H |
| ATOM | 983 | 1HH2 | ARG A | 70161.894 | 3.659 | 9.650 | 1.00 | 0.00 H |
| ATOM | 984 | 2HH2 | ARG A | 70162.443 | 4.738 | 10.889 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.370 | 7.446 | 4.052 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71156.214 | 8.246 | 4.439 | 1.00 | 0.00 C |
| ATOM · | 987 | C | TYR A | 71155.763 | 7.901 | 5.855 | 1.00 | 0.00 C |
| ATOM | 988 | O | TYR A | 71155.335 | 8.772 | 6.611 | 1.00 | 0.00 O |
| ATOM | 989 | CB | TYR A | 71155.062 | 8.026 | 3.457 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.320 | 8.599 | 2.082 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.325 | 7.783 | 0.958 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.557 | 9.957 | 1.908 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.560 | 8.303 | -0.301 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.793 | 10.485 | 0.652 | 1.00 | 0.00 C |
| ATOM | 995 | $C_{i}Z$ | TYR A | 71155.794 | 9.654 | -0.448 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71156.028 | 10.176 | -1.700 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.233 | 6.523 | 3.751 | 1.00 | 0.00 H |
| ATOM | 998 | HA | TYR A | 71156.506 | 9.285 | 4.410 | 1.00 | 0.00 H |
| ATOM | 999 | 1HB | TYR A | 71154.891 | 6.965 | 3.347 | 1.00 | 0.00 H |

| ATOM | 1000 2 | HB | TYR A | 71154.170 | 8.491 | 3.849 | 1.00 | 0.00 H |
|--------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1001 | HD1 | TYR A | 71155.142 | 6.725 | 1.076 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.557 | 10.605 | 2.772 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.561 | 7.653 | -1.163 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.976 | 11.543 | 0.538 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71155.312 | 9.928 | -2.289 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72155.865 | 6.623 | 6.207 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.467 | 6.162 | 7.533 | 1.00 | 0.00 C |
| ATOM - | 1008 | C | PHE A | 72156.458 | 5.134 | 8.069 | 1.00 | 0.00 C |
| ATOM | 1009 | О | PHE A | 72157.415 | 4.764 | 7.388 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72154.063 | 5.558 | 7.486 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72153.887 | 4.530 | 6.405 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72153.603 | 4.914 | 5.104 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72154.006 | 3.179 | 6.690 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72153.441 | 3.971 | 4.108 | 1.00 | 0.00 C |
| ATOM | 1015 | CE2 | PHE A | 72153.844 | 2.231 | 5.697 | 1.00 | 0.00 C |
| ATOM | 1016 | CZ | PHE A | 72153.562 | 2.628 | 4.405 | 1.00 | 0.00 C |
| ATOM | 1017 | Н | PHE A | 72156.214 | 5.975 | 5.561 | 1.00 | 0.00 H |
| ATOM | 1018 | НА | PHE A | 72155.461 | 7.017 | 8.192 | 1.00 | 0.00 H |
| ATOM | 1019 | IНВ | PHE A | 72153.851 | 5.084 | 8.432 | 1.00 | 0.00 H |
| ATOM | 1020 2 | 2HB | PHE A | 72153.345 | 6.348 | 7.315 | 1.00 | 0.00 H |
| ATOM | 1021 | HD1 | PHE A | 72153.509 | 5.965 | 4.871 | 1.00 | 0.00 H |
| ATOM | 1022 | HD2 | PHE A | 72154.227 | 2.868 | 7.700 | 1.00 | 0.00 H |
| ATOM | 1023 | HE1 | PHE A | 72153.219 | 4.284 | 3.097 | 1.00 | 0.00 H |
| ATOM | 1024 | HE2 | PHE A | 72153.939 | 1.181 | 5.932 | 1.00 | 0.00 H |
| ATOM | 1025 | HZ | PHE A | 72153.435 | 1.888 | 3.628 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73156.221 | 4.676 | 9.294 | 1.00 | 0.00 N |

| ATOM | 1027 | CA | THR A | 73157.093 | 3.690 | 9.923 | 1.00 | 0.00 C | |
|------|------|------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 1028 | C | THR A | 73156.375 | 2.353 | 10.085 | 1.00 | 0.00 C | |
| ATOM | 1029 | О | THR A | 73155.407 | 2.245 | 10.838 | 1.00 | 0.00 O | |
| ATOM | 1030 | CB | THR A | 73157.569 | 4.194 | 11.287 | 1.00 | 0.00 C | |
| ATOM | 1031 | OG1 | THR A | 73157.769 | 5.596 | 11.260 | 1.00 | 0.00 O | |
| ATOM | 1032 | CG2 | THR A | 73158.861 | 3.554 | 11.744 | 1.00 | 0.00 C | |
| ATOM | 1033 | Н | THR A | 73155.443 | 5.008 | 9.787 | 1.00 | 0.00 H | |
| ATOM | 1034 | НА | THR A | 73157.950 | 3.549 | 9.283 | 1.00 | 0.00 H | |
| ATOM | 1035 | HB | THR A | 73156.810 | 3.974 | 12.025 | 1.00 | 0.00 H | |
| ATOM | 1036 | HG1 | THR A | 73158.374 | 5.820 | 10.549 | 1.00 | 0.00 H | |
| ATOM | 1037 | 1HG2 | THR A | 73158.644 | 2.615 | 12.232 | 1.00 | 0.00 H | |
| ATOM | 1038 | 2HG2 | THR A | 73159.362 | 4.213 | 12.438 | 1.00 | 0.00 H | |
| ATOM | 1039 | 3HG2 | THR A | 73159.498 | 3.378 | 10.890 | 1.00 | 0.00 H | |
| ATOM | 1040 | N | CYS A | 74156.856 | 1.339 | 9.374 | 1.00 | 0.00 N | |
| ATOM | 1041 | CA | CYS A | 74156.259 | 0.010 | 9.438 | 1.00 | 0.00 C | |
| ATOM | 1042 | С | CYS A | 74157.337 | -1.069 | 9.474 | 1.00 | 0.00 C | |
| ATOM | 1043 | O | CYSA | 74158.530 | -0.770 | 9.420 | 1.00 | 0.00 O | |
| ATOM | 1044 | СВ | CYS A | 74155.333 | -0.215 | 8.241 | 1.00 | 0.00 C | |
| ATOM | 1045 | SG | CYS A | 74153.621 | 0.290 | 8.527 | 1.00 | 0.00 S | |
| ATOM | 1046 | Н | CYS A | 74157.629 | 1.488 | 8.790 | 1.00 | 0.00 H | |
| ATOM | 1047 | НА | CYS A | 74155.679 | -0.049 | 10.346 | 1.00 | 0.00 H | |
| ATOM | 1048 | 1HB | CYS A | 74155.705 | 0.347 | 7.398 | 1.00 | 0.00 H | |
| ATOM | 1049 | 2HB | CYS A | 74155.329 | -1.267 | 7.992 | 1.00 | 0.00 H | |
| ATOM | 1050 | HG | CYS A | 74153.631 | 1.051 | 9.113 | 1.00 | 0.00 H | |
| ATOM | 1051 | N | ALA A | 75156.908 | -2.324 | 9.562 | 1.00 | 0.00 N | |
| ATOM | 1052 | CA | ALA A | 75157.836 | -3.447 | 9.604 | 1.00 | 0.00 C | |
| ATOM | 1053 | C | ALA A | 75158.524 | -3.641 | 8.257 | 1.00 | 0.00 Č | |

| ATOM | 1054 O | ALA A | 75158.192 | -2.974 | 7.277 | 1.00 | 0.00 O |
|--------|-----------|-------|-----------|--------|--------|------|---------------------|
| ATOM | 1055 CB | ALA A | 75157.108 | -4.718 | 10.014 | 1.00 | 0.00 C |
| ATOM | 1056 H | ALA A | 75155.945 | -2.498 | 9.601 | 1.00 | 0.00 H |
| ATOM | 1057 HA | ALA A | 75158.586 | -3.232 | 10.352 | 1.00 | 0.00 H |
| ATOM | 1058 1HB | ALA A | 75156.868 | -5.295 | 9.134 | 1.00 | 0.00 H |
| ATOM | 1059 2HB | ALA A | 75156.197 | -4.459 | 10.535 | 1.00 | 0.00 H |
| ATOM | 1060 3HB | ALA A | 75157.741 | -5.301 | 10.666 | 1.00 | 0.00 H |
| ATOM | 1061 N | LEU A | 76159.485 | -4.558 | 8.216 | 1.00 | 0.00 N |
| ATOM | 1062 CA | LEU A | 76160.222 | -4.840 | 6.989 | 1.00 | 0.00 C |
| ATOM | 1063 C | LEU A | 76159.471 | -5.846 | 6.123 | 1.00 | 0.00 C |
| ATOM | 1064 O | LEU A | 76158.917 | -6.822 | 6.628 | 1.00 | 0.00 ₀ O |
| ATOM | 1065 CB | LEU A | 76161.617 | -5.374 | 7.317 | 1.00 | 0.00 C |
| ATOM | 1066 CG | LEU A | 76162.644 | -4.307 | 7.700 | 1.00 | 0.00 C |
| ATOM | 1067 CD1 | LEU A | 76163.639 | -4.860 | 8.709 | 1.00 | 0.00 C |
| ATOM | 1068 CD2 | LEU A | 76163.367 | -3.795 | 6.463 | 1.00 | 0.00 C |
| ATOM | 1069 H | LEU A | 76159.706 | -5.056 | 9.031 | 1.00 | 0.00 H |
| ATOM | 1070 HA | LEU A | 76160.320 | -3.914 | 6.442 | 1.00 | 0.00 H |
| ATOM | 1071 1HB | LEU A | 76161.529 | -6.070 | 8.139 | 1.00 | 0.00 H |
| ATOM | 1072 2HB | LEU A | 76161.988 | -5.905 | 6.455 | 1.00 | 0.00 H |
| ATOM | 1073 HG | LEU A | 76162.134 | -3.472 | 8.159 | 1.00 | 0.00 H |
| ATOM · | 1074 1HD1 | LEU A | 76163.261 | -4.706 | 9.709 | 1.00 | 0.00 H |
| ATOM | 1075 2HD1 | LEU A | 76164.585 | -4.352 | 8.600 | 1.00 | 0.00 H |
| ATOM | 1076 3HD1 | LEU A | 76163.777 | -5.919 | 8.536 | 1.00 | 0.00 H |
| ATOM | 1077 1HD2 | LEU A | 76162.751 | -3.963 | 5.592 | 1.00 | 0.00 H |
| ATOM | 1078 2HD2 | LEU A | 76164.302 | -4.323 | 6.349 | 1.00 | 0.00 H |
| ATOM | 1079 3HD2 | LEU A | 76163.560 | -2.739 | 6.570 | 1.00 | 0.00 H |
| ATOM | 1080 N | LYS A | 77159.456 | -5.600 | 4.817 | 1.00 | 0.00 N |

| ATOM | 1081 C | A LYS A | 77158.773 | -6.486 | 3.881 | 1.00 | 0.00 C | |
|------|----------|---------|-----------|--------|--------|------|--------|--|
| ATOM | 1082 C | LYS A | 77157.282 | -6.563 | 4.193 | 1.00 | 0.00 C | |
| ATOM | 1083 O | LYS A | 77156.676 | -7.632 | 4.119 | 1.00 | 0.00 O | |
| ATOM | 1084 C | B LYSA | 77159.390 | -7.885 | 3.928 | 1.00 | 0.00 C | |
| ATOM | 1085 C | G LYSA | 77160.875 | -7.906 | 3.603 | 1.00 | 0.00 C | |
| ATOM | 1086 C | D LYS A | 77161.118 | -7.884 | 2.103 | 1.00 | 0.00 C | |
| ATOM | 1087 C | E LYSA | 77162.543 | -7.467 | 1.776 | 1.00 | 0.00 C | |
| ATOM | 1088 N | Z LYS A | 77163.090 | -8.220 | 0.614 | 1.00 | 0.00 N | |
| ATOM | 1089 H | LYS A | 77159.916 | -4.805 | 4.475 | 1.00 | 0.00 H | |
| ATOM | 1090 H | A LYS A | 77158.900 | -6.079 | 2.889 | 1.00 | 0.00 H | |
| ATOM | 1091 1HI | B LYS A | 77159.255 | -8.293 | 4.918 | 1.00 | 0.00 H | |
| ATOM | 1092 2HI | B LYSA | 77158.879 | -8.515 | 3.215 | 1.00 | 0.00 H | |
| ATOM | 1093 1H | G LYSA | 77161.343 | -7.040 | 4.047 | 1.00 | 0.00 H | |
| ATOM | 1094 2H | G LYSA | 77161.311 | -8.804 | 4.017 | 1.00 | 0.00 H | |
| ATOM | 1095 1H | D LYSA | 77160.944 | -8.872 | 1.705 | 1.00 | 0.00 H | |
| ATOM | 1096 2H | D LYSA | 77160.434 | -7.183 | 1.648 | 1.00 | 0.00 H | |
| ATOM | 1097 1H | E LYSA | 77162.551 | -6.412 | 1.544 | 1.00 | 0.00 H | |
| ATOM | 1098 2H | E LYSA | 77163.166 | -7.649 | 2.639 | 1.00 | 0.00 H | |
| ATOM | 1099 1H | Z LYS A | 77162.550 | -7.995 | -0.246 | 1.00 | 0.00 H | |
| ATOM | 1100 2H | Z LYSA | 77163.028 | -9.244 | 0.790 | 1.00 | 0.00 H | |
| ATOM | 1101 3H | Z LYSA | 77164.088 | -7.967 | 0.461 | 1.00 | 0.00 H | |
| ATOM | 1102 N | LYS A | 78156.696 | -5.423 | 4.544 | 1.00 | 0.00 N | |
| ATOM | 1103 C | A LYS A | 78155.275 | -5.362 | 4.868 | 1.00 | 0.00 C | |
| ATOM | 1104 C | LYS A | 78154.692 | -4.001 | 4.500 | 1.00 | 0.00 C | |
| ATOM | 1105 O | LYS A | 78153.843 | -3.465 | 5.212 | 1.00 | 0.00 O | |
| ATOM | 1106 C | B LYS A | 78155.058 | -5.638 | 6.357 | 1.00 | 0.00 C | |
| ATOM | 1107 C | G LYS A | 78155.577 | -6.994 | 6.806 | 1.00 | 0.00 C | |

| ATOM | 1100 | CD | IVCA | 79155 201 | 7 224 | 8.282 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1108 | CD | LYSA | 78155.301 | -7.234 | | | |
| ATOM | 1109 | CE | LYS A | 78154.066 | -8.098 | 8.483 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78153.349 | -7.755 | 9.743 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.232 | -4.604 | 4.586 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.772 | -6.123 | 4.293 | 1.00 | 0.00 H |
| ATOM | 1113 1 | НВ | LYS A | 78155.565 | -4.875 | 6.930 | 1.00 | 0.00 H |
| ATOM | 11142 | 2HB | LYS A | 78154.001 | -5.592 | 6.569 | 1.00 | 0.00 H |
| ATOM | 1115 1 | HG | LYS A | 78155.089 | -7.764 | 6.228 | 1.00 | 0.00 H |
| ATOM | 1116 2 | HG | LYS A | 78156.643 | -7.035 | 6.636 | 1.00 | 0.00 H |
| ATOM | 1117 1 | HD | LYS A | 78156.152 | -7.734 | 8.720 | 1.00 | 0.00 H |
| ATOM | 1118 2 | 2HD | LYS A | 78155.148 | -6.283 | 8.769 | 1.00 | 0.00 H |
| ATOM | 1119 1 | HE | LYS A | 78153.399 | -7.950 | 7.649 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYS A | 78154.369 | -9.134 | 8.522 | 1.00 | 0.00 H |
| ATOM | 1121 | ΙHΖ | LYS A | 78152.922 | -8.610 | 10.155 | 1.00 | 0.00 H |
| ATOM | 1122 2 | 2HZ | LYS A | 78152.597 | -7.065 | 9.549 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYS A | 78154.012 | -7.345 | 10.431 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.152 | -3.448 | 3.382 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.674 | -2.151 | 2.920 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.599 | -2.103 | 1.397 | 1.00 | 0.00 C |
| ATOM | 1127 | O | ALA A | 79155.621 | -2.002 | 0.719 | 1.00 | 0.00 O |
| ATOM | 1128 | СВ | ALA A | 79155.576 | -1.041 | 3.440 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79155.828 | -3.923 | 2.856 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.684 | -1.996 | 3.324 | 1.00 | 0.00 H |
| ATOM | 1131 | 1HB | ALA A | 79155.178 | -0.659 | 4.369 | 1.00 | 0.00 H |
| ATOM | 1132 | 2HB | ALA A | 79155.621 | -0.243 | 2.714 | 1.00 | 0.00 H |
| ATOM | 1133 | 3HB | ALA A | 79156.569 | -1.432 | 3.607 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.382 | -2.177 | 0.868 | 1.00 | 0.00 N |
| | | | | | | | | |

| ATOM | 1135 | CA | LEU A | 80153.172 | -2.143 | -0.576 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1136 | C | LEU A | 80152.306 | -0.951 | -0.970 | 1.00 | 0.00 C |
| ATOM | 1137 | О | LEU A | 80151.157 | -0.836 | -0.541 | 1.00 | 0.00 O |
| ATOM | 1138 | CB | LEU A | 80152.518 | -3.443 | -1.047 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.189 | -3.497 | -2.540 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.449 | -3.741 | -3.356 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80151.155 | -4.579 | -2.817 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.606 | -2.257 | 1.462 | 1.00 | 0.00 H |
| ATOM | 1143 | HA | LEU A | 80154.137 | -2.043 | -1.049 | 1.00 | 0.00 H |
| ATOM | 1144 | 1HB | LEU A | 80153.185 | -4.261 | - 0.816 | 1.00 | 0.00 H |
| ATOM | 1145 | 2HB | LEU A | 80151.601 | -3.581 | -0.494 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.772 | -2.549 | -2.845 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | LEU A | 80153.391 | -3.188 | -4.282 | 1.00 | 0.00 H |
| ATOM | 1148 | 2HD1 | LEU A | 80153.541 | - 4.794 | -3.571 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80154.311 | -3.411 | -2.794 | 1.00 | 0.00 H |
| ATOM | 1150 | 1HD2 | LEU A | 80150.553 | -4.292 | -3.666 | 1.00 | 0.00 H |
| ATOM | 1151 | 2HD2 | LEU A | 80150.522 | -4.703 | -1.951 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80151.658 | -5.511 | -3.032 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.863 | -0.066 | -1.789 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.142 | 1.118 | -2.242 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.299 | 0.803 | -3.473 | 1.00 | 0.00 C |
| ATOM | 1156 | О | PHE A | 81151.736 | 0.083 | -4.371 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.123 | 2.249 | -2.557 | 1.00 | 0.00 C |
| ATOM | 1158 | CĠ | PHE A | 81153.763 | 2.847 | -1.336 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81153.243 | 3.993 | -0.757 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81154.883 | 2.260 | -0.768 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81153.829 | 4.545 | 0.367 | 1.00 | 0.00 C |

2.808 0.355 1.00 0.00 C CE2 PHE A 81155.473 **ATOM** 1162 3.952 0.923 1.00 0.00 C CZ PHE A 81154.946 **ATOM** 1163 -0.212 -2.096 1.00 0.00 H**ATOM** 1164 Н PHE A 81153.783 -1.443 1.00 0.00 H1165 HA PHE A 81151.487 1.433 **ATOM** 1166 1HB PHE A 81153.910 1.868 -3.191 1.00 0.00 H**ATOM** -3.077 1.00 0.00 H**ATOM** 1167 2HB PHE A 81152.597 3.037 -1.1901.00 0.00 H1168 HD1 PHE A 81152.370 4.457 **ATOM** HD2 PHE A 81155.296 1.367 -1.212 1.00 0.00 H **ATOM** 1169 5.439 0.809 1.00 0.00 H 1170 HE1 PHE A 81153.416 **ATOM** 2.343 0.788 1.00 0.00 H HE2 PHE A 81156.346 **ATOM** 1171 **ATOM** 1172 HZ PHE A 81155.407 4.381 1.802 1.00 0.00 H 1.00 0.00 N 1.347 -3.509 **ATOM** 1173 N **VALA** 82150.087 **VALA** 82149.182 1.124 -4.631 1.00 0.00 C 1174 CA **ATOM** -4.873 1.00 0.00 C VALA 82148.297 2.342 **ATOM** 1175 \mathbf{C} 1.00 0.00 O **VALA** 82148.200 3.229 -4.027 **ATOM** 1176 0 1.00 0.00 C **ATOM** 1177 CB **VALA** 82148.288 -0.107 -4.394 -4.425 82149.115 1.00 0.00 C **ATOM** 1178 CG1 VAL A -1.382 0.021 -3.0771.00 0.00 C CG2 VAL A 82147.539 **ATOM** 1179 -2.7641.00 0.00 H **ATOM** 1180 Η VAL A 82149.794 1.912 1.00 0.00 H 0.945 -5.512 HA VAL A 82149.780 **ATOM** 1181 1.00 0.00 H 1182 HB VAL A 82147.561 -0.158 -5.192 **ATOM** -1.499 -5.401 1.00 0.00 H 1183 1HG1 VAL A 82149.562 **ATOM** 1.00 0.00 H1184 2HG1 VAL A 82148.478 -2.230 -4.217 **ATOM** 1.00 0.00 H 1185 3HG1 VALA 82149.893 -1.325 -3.677 **ATOM** 1.00 0.00 H 1186 1HG2 VAL A 82147.408 -0.959 -2.641**ATOM** 1.00 0.00 H 1187 2HG2 VALA 82146.572 0.469 -3.254 **ATOM** 1.00 0.00 H -2.400 1188 3HG2 VAL A 82148.106 0.644 **ATOM**

| ATOM | 1189 | N | LYS A | 83147.652 | 2.375 | -6.035 | 1.00 | 0.00 N |
|-------------------|--------|----|-------|-----------|----------|--------|------|--------|
| ATOM | 1190 | CA | LYS A | 83146.774 | 3.484 | -6.390 | 1.00 | 0.00 C |
| ATOM | 1191 | C | LYS A | 83145.517 | 3.482 | -5.528 | 1.00 | 0.00 C |
| ATOM | 1192 | O | LYS A | 83144.750 | 2.518 | -5.530 | 1.00 | 0.00 O |
| ATOM | 1193 | СВ | LYS A | 83146.392 | 3.406 | -7.870 | 1.00 | 0.00 C |
| ATOM | 1194 | CG | LYS A | 83147.588 | 3.405 | -8.808 | 1.00 | 0.00 C |
| ATOM | 1195 | CD | LYS A | 83147.168 | 3.152 - | 10.247 | 1.00 | 0.00 C |
| ATOM | 1196 | CE | LYS A | 83147.976 | 3.993 - | 11.220 | 1.00 | 0.00 C |
| ATOM | 1197 | NZ | LYS A | 83148.286 | 3.250 - | 12.472 | 1.00 | 0.00 N |
| ATOM | 1198 | Н | LYS A | 83147.770 | 1.637 | -6.669 | 1.00 | 0.00 H |
| ATOM | 1199 | НА | LYS A | 83147.313 | 4.403 | -6.216 | 1.00 | 0.00 H |
| ATOM | 1200 1 | НВ | LYS A | 83145.830 | 2.498 | -8.038 | 1.00 | 0.00 H |
| ATOM | 1201 2 | НВ | LYS A | 83145.770 | 4.254 | -8.115 | 1.00 | 0.00 H |
| ATOM | 1202 1 | HG | LYS A | 83148.078 | 4.366 | -8.751 | 1.00 | 0.00 H |
| ATOM | 1203 2 | HG | LYS A | 83148.274 | 2.630 | -8.501 | 1.00 | 0.00 H |
| ATOM [*] | 1204 1 | HD | LYS A | 83147.318 | 2.108 - | 10.477 | 1.00 | 0.00 H |
| ATOM | 1205 2 | HD | LYS A | 83146.121 | 3.398 - | 10.354 | 1.00 | 0.00 H |
| ATOM | 1206 1 | HE | LYS A | 83147.410 | 4.879 -1 | 1.469 | 1.00 | 0.00 H |
| ATOM | 1207 2 | HE | LYS A | 83148.902 | 4.282 -1 | 10.744 | 1.00 | 0.00 H |
| ATOM | 1208 1 | HZ | LYS A | 83149.234 | 3.508 -1 | 12.816 | 1.00 | 0.00 H |
| ATOM | 1209 2 | HZ | LYS A | 83147.589 | 3.481 - | 13.207 | 1.00 | 0.00 H |
| ATOM | 1210 3 | HZ | LYS A | 83148.261 | 2.226 - | 12.296 | 1.00 | 0.00 H |
| ATOM | 1211 | N | LEU A | 84145.313 | 4.569 | -4.792 | 1.00 | 0.00 N |
| ATOM | 1212 | CA | LEU A | 84144.151 | 4.700 | -3.922 | 1.00 | 0.00 C |
| ATOM | 1213 | C | LEU A | 84142.856 | 4.573 | -4.719 | 1.00 | 0.00 C |
| ATOM | 1214 | О | LEU A | 84141.863 | 4.038 | -4.227 | 1.00 | 0.00 O |
| ATOM | 1215 | CB | LEU A | 84144.189 | 6.045 | -3.194 | 1.00 | 0.00 C |

| ATOM | 1216 | CG | LEU A | 84142.978 | 6.339 | -2.308 | 1.00 | 0.00 C |
|------|--------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1217 | CD1 | LEU A | 84143.141 | 5.682 | -0.946 | 1.00 | 0.00 C |
| ATOM | 1218 | CD2 | LEU A | 84142.780 | 7.840 | -2.158 | 1.00 | 0.00 C |
| ATOM | 1219 | Н | LEU A | 84145.962 | 5.301 | -4.836 | 1.00 | 0.00 H |
| ATOM | 1220 | НА | LEU A | 84144.191 | 3.905 | -3.193 | 1.00 | 0.00 H |
| ATOM | 1221 | IНВ | LEU A | 84145.075 | 6.071 | -2.577 | 1.00 | 0.00 H |
| ATOM | 1222 | 2HB | LEU A | 84144.264 | 6.827 | -3.934 | 1.00 | 0.00 H |
| ATOM | 1223 | HG | LEU A | 84142.091 | 5.928 | -2.771 | 1.00 | 0.00 H |
| ATOM | 1224 | 1HD1 | LEU A | 84143.630 | 4.727 | -1.063 | 1.00 | 0.00 H |
| ATOM | 1225 | 2HD1 | LEU A | 84142.169 | 5.537 | -0.497 | 1.00 | 0.00 H |
| ATOM | 1226 | 3HD1 | LEU A | 84143.739 | 6.318 | -0.309 | 1.00 | 0.00 H |
| ATOM | 1227 | 1HD2 | LEU A | 84141.894 | 8.030 | -1.571 | 1.00 | 0.00 H |
| ATOM | 1228 2 | 2HD2 | LEU A | 84142.667 | 8.287 | -3.134 | 1.00 | 0.00 H |
| ATOM | 1229 | 3HD2 | LEU A | 84143.639 | 8.268 | -1.663 | 1.00 | 0.00 H |
| ATOM | 1230 | N | LYS A | 85142.875 | 5.070 | -5.951 | 1.00 | 0.00 N |
| ATOM | 1231 | CA | LYS A | 85141.701 | 5.014 | -6.815 | 1.00 | 0.00 C |
| ATOM | 1232 | C | LYS A | 85141.332 | 3.569 | -7.138 | 1.00 | 0.00 C |
| ATOM | 1233 | O | LYS A | 85140.173 | 3.263 | -7.421 | 1.00 | 0.00 O |
| ATOM | 1234 | СВ | LYS A | 85141.958 | 5.788 | -8.109 | 1.00 | 0.00 C |
| ATOM | 1235 | CG | LYS A | 85143.098 | 5.223 | -8.941 | 1.00 | 0.00 C |
| ATOM | 1236 | CD | LYS A | 85143.604 | 6.236 | -9.955 | 1.00 | 0.00 C |
| ATOM | 1237 | CE | LYS A | 85144.941 | 5.817 - | 10.542 | 1.00 | 0.00 C |
| ATOM | 1238 | NZ | LYS A | 85145.553 | 6.900 | -11.362 | 1.00 | 0.00 N |
| ATOM | 1239 | Н | LYS A | 85143.696 | 5.486 | -6.287 | 1.00 | 0.00 H |
| ATOM | 1240 | НА | LYS A | 85140.879 | 5.473 | -6.289 | 1.00 | 0.00 H |
| ATOM | 1241 | 1HB | LYS A | 85141.060 | 5.770 | -8.710 | 1.00 | 0.00 H |
| ATOM | 1242 | 2HB | LYS A | 85142.195 | 6.812 | -7.862 | 1.00 | 0.00 H |

| ATOM | 1243 1 | HG | LYS A | 85143.910 | 4.952 | -8.283 | 1.00 | 0.00 H |
|------|--------|----|-------|-----------|----------|--------|------|--------|
| ATOM | 1244 2 | HG | LYS A | 85142.748 | 4.346 | -9.465 | 1.00 | 0.00 H |
| ATOM | 1245 1 | HD | LYS A | 85142.882 | 6.323 - | 10.753 | 1.00 | 0.00 H |
| ATOM | 1246 2 | HD | LYS A | 85143.719 | 7.193 | -9.466 | 1.00 | 0.00 H |
| ATOM | 1247 1 | HE | LYS A | 85145.613 | 5.567 | -9.734 | 1.00 | 0.00 H |
| ATOM | 1248 2 | HE | LYS A | 85144.790 | 4.948 -1 | 1.165 | 1.00 | 0.00 H |
| ATOM | 1249 1 | HZ | LYS A | 85145.891 | 7.666 -1 | 0.746 | 1.00 | 0.00 H |
| ATOM | 1250 2 | HZ | LYS A | 85144.850 | 7.287 -1 | 12.023 | 1.00 | 0.00 H |
| ATOM | 1251 3 | HZ | LYS A | 85146.356 | 6.526 -1 | 11.906 | 1.00 | 0.00 H |
| ATOM | 1252 | N | SER A | 86142.322 | 2.682 | -7.094 | 1.00 | 0.00 N |
| ATOM | 1253 | CA | SER A | 86142.098 | 1.271 | -7.381 | 1.00 | 0.00 C |
| ATOM | 1254 | C | SER A | 86142.057 | 0.453 | -6.095 | 1.00 | 0.00 C |
| ATOM | 1255 | O | SER A | 86142.443 | -0.716 | -6.079 | 1.00 | 0.00 O |
| ATOM | 1256 | CB | SER A | 86143.194 | 0.737 | -8.305 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.269 | 1.496 | -9.499 | 1.00 | 0.00 O |
| ATOM | 1258 | H | SER A | 86143.225 | 2.984 | -6.862 | 1.00 | 0.00 H |
| ATOM | 1259 | НА | SER A | 86141.144 | 1.182 | -7.881 | 1.00 | 0.00 H |
| ATOM | 1260 1 | НВ | SER A | 86144.146 | 0.792 | -7.799 | 1.00 | 0.00 H |
| ATOM | 1261 2 | HB | SER A | 86142.980 | -0.290 | -8.558 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86142.385 | 1.639 | -9.845 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.587 | 1.075 | -5.018 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.496 | 0.404 | -3.726 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87140.043 | 0.114 | -3.366 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYSA | 87139.125 | 0.737 | -3.901 | 1.00 | 0.00 O |
| ATOM | 1267 | CB | CYS A | 87142.143 | 1.260 | -2.637 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYS A | 87143.948 | 1.167 | -2.600 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYSA | 87141.296 | 2.007 | -5.094 | 1.00 | 0.00 H |

0.00 H -0.532 -3.8011.00 **ATOM** 1270 HA CYS A 87142.029 -2.7921.00 0.00 HCYS A 87141.871 2.293 1271 1HB **ATOM** CYS A 87141.777 0.938 - 1.673 1.00 0.00 H 1272 2HB **ATOM** 1.809 -1.959 1.00 0.00 HCYS A 87144.265 **ATOM** 1273 HG -0.834 -2.4581.00 0.00 N 88139.840 1274 N ARG A **ATOM** 0.00 C 1275 CAARG A 88138.497 -1.205-2.0281.00 **ATOM** -0.503 1.00 0.00 C 88138.413 - 1.271 \mathbf{C} ARG A **ATOM** 1276 -1.8260.151 1.00 0.00 O **ARGA** 88139.296 **ATOM** 1277 0 -2.631 1.00 0.00 C 88138.102 -2.555**ATOM** 1278 CBARG A -3.921 1.00 0.00 C 88137.308 -2.435 CG ARG A **ATOM** 1279 1280 CD ARG A 88135.810 -2.459-3.658 1.00 0.00 C **ATOM** -4.778 1.00 0.00 N 1281 NE ARG A 88135.049 -1.912 **ATOM** -1.490 -4.682 1.00 0.00 C **ARGA** 88133.789 1282 CZ**ATOM** -3.522 1.00 0.00 N 1283 NH1 ARG A 88133.148 -1.550 **ATOM** -1.005 -5.749 1.00 0.00 N 88133.171 1284 NH2 ARG A **ATOM** ARG A 88140.612 -1.296 -2.068 1.00 0.00 H 1285 Η **ATOM** -0.449 0.00 H**ARG A** 88137.816 -2.386 1.00 **ATOM** 1286 HA 0.00 H -3.121 -2.8361.00 **ATOM** 1287 1HB ARG A 88138.998 0.00 H 1288 2HB ARG A 88137.502 -3.096 -1.9141.00 **ATOM** 1.00 0.00 H 88137.563 -1.504 -4.4051289 1HG **ARG A ATOM** 88137.564 -3.262 -4.568 1.00 0.00 H 1290 2HG **ARG A ATOM** -3.491 1.00 0.00 H ARG A 88135.504 -3.481 **ATOM** 1291 1HD ARG A 88135.604 -1.873 -2.7731.00 0.00 H1292 2HD **ATOM** ARG A 88135.498 -1.856 -5.647 1.00 0.00 H**ATOM** 1293 HE 0.00 H-1.915-2.7131.00 1294 1HH1 ARG A 88133.608 **ATOM** 1.00 0.00 H 1295 2HH1 ARG A 88132.203 -1.231 -3.456 **ATOM** 0.00 H -0.958-6.626 1.00 **ATOM** 1296 1HH2 ARG A 88133.649

| ATOM | 1297 2 | 2HH2 | ARG A | 88132.225 | -0.688 | -5.678 | 1.00 | 0.00 H |
|------|--------|------|---------|-----------|--------|--------|------|--------|
| ATOM | 1298 | N | PRO A | 89137.344 | -0.704 | 0.089 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89137.157 | -0.707 | 1.544 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.223 | -2.113 | 2.132 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.564 | -3.031 | 1.646 | 1.00 | 0.00 O |
| ATOM | 1302 | СВ | PRO A | 89135.757 | -0.117 | 1.729 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.519 | 0.693 | 0.503 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89136.239 | -0.019 | -0.608 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.884 | -0.079 | 2.037 | 1.00 | 0.00 H |
| ATOM | 1306 | HB | PRO A | 89135.037 | -0.916 | 1.822 | 1.00 | 0.00 H |
| ATOM | 1307 2 | 2HB | PRO A | 89135.737 | 0.498 | 2.617 | 1.00 | 0.00 H |
| ATOM | 1308 | IHG | PRO A | 89134.461 | 0.740 | 0.294 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89135.922 | 1.686 | 0.635 | 1.00 | 0.00 H |
| ATOM | 1310 | IHD | PRO A | 89135.584 | -0.732 | -1.086 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89136.619 | 0.691 | -1.326 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASP A | 90138.021 | -2.273 | 3.183 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASPA | 90138.172 | -3.568 | 3.838 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASP A | 90137.378 | -3.612 | 5.140 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASP A | 90137.759 | -2.992 | 6.133 | 1.00 | 0.00 O |
| ATOM | 1316 | СВ | ASPA | 90139.648 | -3.854 | 4.116 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90139.948 | -5.339 | 4.174 | 1.00 | 0.00 C |
| ATOM | 1318 | ODI | ASPA | 90140.366 | -5.819 | 5.248 | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | 2 ASP A | 90139.764 | -6.022 | 3.144 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASP A | 90138.520 | -1.503 | 3.526 | 1.00 | 0.00 H |
| ATOM | 1321 | НА | ASPA | 90137.787 | -4.323 | 3.170 | 1.00 | 0.00 H |
| ATOM | 1322 | 1HB | ASPA | 90140.247 | -3.414 | 3.333 | 1.00 | 0.00 H |
| ATOM | 1323 | 2HB | ASPA | 90139.921 | -3.412 | 5.063 | 1.00 | 0.00 H |

| ATOM | 1324 | N | SER A | 91136.274 | -4.352 | 5.129 | 1.00 | 0.00 N |
|------|--------|-----|-------|-----------|---------|-------|------|--------|
| ATOM | 1325 | CA | SER A | 91135.426 | -4.478 | 6.310 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91135.724 | -5.774 | 7.057 | 1.00 | 0.00 C |
| ATOM | 1327 | O | SER A | 91134.840 | -6.355 | 7.688 | 1.00 | 0.00 O |
| ATOM | 1328 | СВ | SER A | 91133.950 | -4.434 | 5.911 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91133.158 | -3.879 | 6.947 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91136.023 | -4.823 | 4.308 | 1.00 | 0.00 H |
| ATOM | 1331 | НА | SER A | 91135.639 | -3.644 | 6.961 | 1.00 | 0.00 H |
| ATOM | 1332 1 | HВ | SER A | 91133.837 | -3.827 | 5.024 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91133.605 | -5.436 | 5.708 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91132.243 | -3.834 | 6.660 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92136.972 | -6.223 | 6.981 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92137.384 | -7.451 | 7.650 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92137.327 | -7.291 | 9.166 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92137.085 | -8.254 | 9.893 | 1.00 | 0.00 O |
| ATOM | 1339 | СВ | ARG A | 92138.798 | -7.842 | 7.220 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92138.835 | -8.741 | 5.995 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92140.147 | -9.503 | 5.902 | 1.00 | 0.00 C |
| ATOM | 1342 | NE | ARG A | 92140.288 | -10.485 | 6.976 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92139.667 | -11.663 | 6.989 | 1.00 | 0.00 C |
| ATOM | 1344 | NHI | ARG A | 92138.865 | -12.010 | 5.991 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92139.851 | -12.496 | 8.004 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92137.632 | -5.717 | 6.462 | 1.00 | 0.00 H |
| ATOM | 1347 | HA | ARG A | 92136.700 | -8.234 | 7.358 | 1.00 | 0.00 H |
| ATOM | 1348 | 1HB | ARG A | 92139.355 | -6.944 | 6.997 | 1.00 | 0.00 H |
| ATOM | 1349 | 2HB | ARG A | 92139.281 | -8.361 | 8.035 | 1.00 | 0.00 H |
| ATOM | 1350 | 1HG | ARG A | 92138.022 | -9.450 | 6.056 | 1.00 | 0.00 H |

| ATOM | 1351 2 | 2HG | ARG A | 92138.719 | -8.133 | 5.109 | 1.00 | 0.00 H |
|------|--------|--------|-------|-------------|---------|--------|------|--------|
| ATOM | 1352 1 | HD | ARG A | 92140.185 | -10.016 | 4.953 | 1.00 | 0.00 H |
| ATOM | 1353 2 | 2HD | ARG A | 92140.963 | -8.798 | 5.962 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92140.875 | -10.253 | 7.725 | 1.00 | 0.00 H |
| ATOM | 1355 1 | IHH1 A | ARG A | 92138.722 - | 11.386 | 5.223 | 1.00 | 0.00 H |
| ATOM | 1356 2 | 2HH1 / | ARG A | 92138.403 - | 12.896 | 6.007 | 1.00 | 0.00 H |
| ATOM | 1357 | HH2 | ARG A | 92140.455 - | 12.240 | 8.758 | 1.00 | 0.00 H |
| ATOM | 1358 2 | 2HH2 / | ARG A | 92139.385 - | 13.381 | 8.014 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93137.554 | -6.068 | 9.637 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93137.528 | -5.782 | 11.067 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93136.525 | -4.678 | 11.385 | 1.00 | 0.00 C |
| ATOM | 1362 | O | PHE A | 93136.707 | -3.917 | 12.335 | 1.00 | 0.00 O |
| ATOM | 1363 | СВ | PHE A | 93138.921 | -5.377 | 11.551 | 1.00 | 0.00 C |
| ATOM | 1364 | CG | PHE A | 93139.888 | -6.524 | 11.626 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93140.464 | -6.884 | 12.834 | 1.00 | 0.00 C |
| ATOM | 1366 | CD2 | PHE A | 93140.221 | -7.243 | 10.489 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93141.354 | -7.938 | 12.907 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93141.111 | -8.298 | 10.555 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ | PHE A | 93141.677 | -8.646 | 11.765 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93137.741 | -5.341 | 9.007 | 1.00 | 0.00 H |
| ATOM | 1371 | HA | PHE A | 93137.227 | -6.684 | 11.579 | 1.00 | 0.00 H |
| ATOM | 1372 | 1HB | PHE A | 93139.330 | -4.642 | 10.874 | 1.00 | 0.00 H |
| ATOM | 1373 | 2HB | PHE A | 93138.839 | -4.945 | 12.537 | 1.00 | 0.00 H |
| ATOM | 1374 | HD1 | PHE A | 93140.212 | -6.330 | 13.727 | 1.00 | 0.00 H |
| ATOM | 1375 | HD2 | PHE A | 93139.778 | -6.971 | 9.543 | 1.00 | 0.00 H |
| ATOM | 1376 | HE1 | PHE A | 93141.796 | -8.208 | 13.854 | 1.00 | 0.00 H |
| ATOM | 1377 | HE2 | PHE A | 93141.361 | -8.850 | 9.662 | 1.00 | 0.00 H |

| ATOM | 1378 | HZ | PHE A | 93142.373 | -9.471 | 11.820 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 1379 | N | ALA A | 94135.467 | -4.596 | 10.586 | 1.00 | 0.00 N |
| ATOM | 1380 | CA | ALA A | 94134.436 | -3.584 | 10.785 | 1.00 | 0.00 C |
| ATOM | 1381 | C | ALA A | 94133.274 | -4.138 | 11.602 | 1.00 | 0.00 C |
| ATOM | 1382 | O | ALA A | 94132.658 | -5.136 | 11.227 | 1.00 | 0.00 O |
| ATOM | 1383 | СВ | ALA A | 94133.940 | -3.064 | ·9.444 | 1.00 | 0.00 C |
| ATOM | 1384 | Н | ALA A | 94135.376 | -5.231 | 9.844 | 1.00 | 0.00 H |
| ATOM | 1385 | НА | ALA A | 94134.879 | -2.759 | 11.322 | 1.00 | 0.00 H |
| ATOM | 1386 1 | lНВ | ALA A | 94133.035 | -3.584 | 9.169 | 1.00 | 0.00 H |
| ATOM | 1387 2 | 2HB | ALA A | 94134.696 | -3.235 | 8.691 | 1.00 | 0.00 H |
| ATOM | 1388 3 | ЗНВ | ALA A | 94133.739 | -2.007 | 9.520 | 1.00 | 0.00 H |
| ATOM | 1389 | N | SER A | 95132.980 | -3.485 | 12.721 | 1.00 | 0.00 N |
| ATOM | 1390 | CA | SER A | 95131.891 | -3.913 | 13.593 | 1.00 | 0.00 C |
| ATOM | 1391 | C | SER A | 95130.740 | -2.913 | 13.557 | 1.00 | 0.00 C |
| ATOM | 1392 | O | SER A | 95130.944 | -1.724 | 13.314 | 1.00 | 0.00 O |
| ATOM | 1393 | CB | SER A | 95132.394 | -4.078 | 15.028 | 1.00 | 0.00 C |
| ATOM | 1394 | OG | SER A | 95131.383 | -4.612 | 15.865 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95133.508 | -2.696 | 12.967 | 1.00 | 0.00 H |
| ATOM | 1396 | HA | SER A | 95131.535 | -4.867 | 13.234 | 1.00 | 0.00 H |
| ATOM | 1397 | 1HB | SER A | 95133.240 | -4.748 | 15.035 | 1.00 | 0.00 H |
| ATOM | 1398 2 | 2HB | SER A | 95132.695 | -3.115 | 15.415 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95131.061 | -5.436 | 15.493 | 1.00 | 0.00 H |
| ATOM | 1400 | N | LEU A | 96129.529 | -3.404 | 13.802 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96128.344 | -2.554 | 13.798 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96127.403 | -2.931 | 14.938 | 1.00 | 0.00 C |
| ATOM | 1403 | О | LEU A | 96126.670 | -3.916 | 14.852 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96127.616 | - 2.665 | 12.456 | 1.00 | 0.00 C |

1.00 0.00 C CG LEU A 96127.763 -1.451 11.537 **ATOM** 1405 1.00 0.00 C CD1 LEU A 96129.230 -1.182 11.239 **ATOM** 1406 -1.664 10.247 1.00 0.00 C **ATOM** 1407 CD2 LEU A 96126.985 -4.361 1.00 0.00 H 96129.430 13.989 **ATOM** 1408 Η LEU A 1409 HA LEU A 96128.669 -1.534 13.938 1.00 0.00 H **ATOM** 11.936 1.00 0.00 H**ATOM** 1410 1HB LEU A 96127.996 -3.533 -2.816 12.649 1.00 0.00 H LEU A 96126.564 **ATOM** 1411 2HB 1412 HG LEUA 96127.358 -0.581 12.034 1.00 0.00 H **ATOM** 11.952 1.00 0.00 H1413 1HD1 LEU A 96129.616 -0.468 **ATOM** -0.782 10.241 1.00 0.00 H 1414 2HD1 LEU A 96129.327 **ATOM ATOM** 1415 3HD1 LEU A 96129.788 -2.103 11.315 1.00 0.00 H-1.959 10.481 1.00 0.00 H**ATOM** 1416 1HD2 LEU A 96125.972 -2.438 9.663 1.00 0.00 H1417 2HD2 LEU A 96127.460 **ATOM** -0.743 9.681 1.00 0.00 H **ATOM** 1418 3HD2 LEU A 96126.969 97127.429 -2.139 16.006 1.00 0.00 N **ATOM** 1419 N GLN A **ATOM** 1420 CA GLN A 97126.577 -2.389 17.163 1.00 0.00 C 17.778 1.00 0.00 C **ATOM** 1421 \mathbf{C} GLN A 97126.881 -3.753 17.433 1.00 0.00 O 97126.251 -4.753 **ATOM** 1422 0 GLN A 16.763 1.00 0.00 C **ATOM** 1423 CB GLN A 97125.102 -2.314 16.001 1.00 0.00 C GLN A 97124.743 -1.048 **ATOM** 1424 CG CD GLN A 97124.686 0.175 16.897 1.00 0.00 C **ATOM** 1425 17.686 1.00 0.00 OOE1 GLN A 97123.756 0.338 **ATOM** 1426 NE2 GLN A 97125.684 1.041 16.778 1.00 0.00 N **ATOM** 1427 0.00 H GLN A 97128.035 -1.369 16.015 1.00 **ATOM** 1428 Η 0.00 H -1.62317.896 1.00 HAGLN A 97126.782 **ATOM** 1429 -3.162 16.139 1.00 0.00 H GLN A 97124.867 **ATOM** 1430 1HB 0.00 H -2.355 17.656 1.00 **ATOM** 1431 2HB GLN A 97124.497

| ATOM | 1432 1HG | GLN A | 97125.485 | -0.880 | 15.236 | 1.00 | 0.00 H |
|------|-----------|-------|-----------|--------|--------|------|--------|
| ATOM | 1433 2HG | GLN A | 97123.775 | -1.184 | 15.540 | 1.00 | 0.00 H |
| ATOM | 1434 1HE2 | GLN A | 97126.392 | 0.846 | 16.128 | 1.00 | 0.00 H |
| ATOM | 1435 2HE2 | GLN A | 97125.673 | 1.841 | 17.345 | 1.00 | 0.00 H |
| ATOM | 1436 N | PRO A | 98127.854 | -3.812 | 18.702 | 1.00 | 0.00 N |
| ATOM | 1437 CA | PRO A | 98128.239 | -5.063 | 19.366 | 1.00 | 0.00 C |
| ATOM | 1438 C | PRO A | 98127.043 | -5.789 | 19.971 | 1.00 | 0.00 C |
| ATOM | 1439 O | PRO A | 98127.044 | -7.014 | 20.094 | 1.00 | 0.00 O |
| ATOM | 1440 CB | PRO A | 98129.197 | -4.602 | 20.467 | 1.00 | 0.00 C |
| ATOM | 1441 CG | PRO A | 98129.755 | -3.315 | 19.969 | 1.00 | 0.00 C |
| ATOM | 1442 CD | PRO A | 98128.656 | -2.668 | 19.173 | 1.00 | 0.00 C |
| ATOM | 1443 HA | PRO A | 98128.755 | -5.726 | 18.689 | 1.00 | 0.00 H |
| ATOM | 1444 1HB | PRO A | 98128.652 | -4.467 | 21.389 | 1.00 | 0.00 H |
| ATOM | 1445 2HB | PRO A | 98129.973 | -5.341 | 20.605 | 1.00 | 0.00 H |
| ATOM | 1446 1HG | PRO A | 98130.034 | -2.688 | 20.803 | 1.00 | 0.00 H |
| ATOM | 1447 2HG | PRO A | 98130.611 | -3.505 | 19.338 | 1.00 | 0.00 H |
| ATOM | 1448 1HD | PRO A | 98128.067 | -2.017 | 19.803 | 1.00 | 0.00 H |
| ATOM | 1449 2HD | PRO A | 98129.067 | -2.117 | 18.340 | 1.00 | 0.00 H |
| ATOM | 1450 N | SER A | 99126.021 | -5.025 | 20.346 | 1.00 | 0.00 N |
| ATOM | 1451 CA | SER A | 99124.818 | -5.596 | 20.940 | 1.00 | 0.00 C |
| ATOM | 1452 C | SER A | 99123.564 | -4.983 | 20.323 | 1.00 | 0.00 C |
| ATOM | 1453 O | SER A | 99123.584 | -3.845 | 19.855 | 1.00 | 0.00 O |
| ATOM | 1454 CB | SER A | 99124.815 | -5.377 | 22.453 | 1.00 | 0.00 C |
| ATOM | 1455 OC | SER A | 99125.417 | -6.469 | 23.127 | 1.00 | 0.00 O |
| ATOM | 1456 H | SER A | 99126.079 | -4.054 | 20.222 | 1.00 | 0.00 H |
| ATOM | 1457 HA | SER A | 99124.820 | -6.657 | 20.738 | 1.00 | 0.00 H |
| ATOM | 1458 1HB | SER A | 99125.367 | -4.479 | 22.686 | 1.00 | 0.00 H |

| ATOM | 1459 2HB | SER A 99123.797 | -5.273 | 22.798 | 1.00 | 0.00 H |
|------|----------|------------------|--------|--------|--------------|--------|
| ATOM | 1460 HG | SER A 99124.734 | -7.021 | 23.516 | 1.00 | 0.00 H |
| ATOM | 1461 N | GLY A 100122.475 | -5.744 | 20.327 | 1.00 | 0.00 N |
| ATOM | 1462 CA | GLY A 100121.229 | -5.258 | 19.766 | 1.00 | 0.00 C |
| ATOM | 1463 C | GLY A 100120.594 | -4.171 | 20.614 | 1.00 | 0.00 C |
| ATOM | 1464 O | GLY A 100120.434 | -3.039 | 20.157 | 1.00 | 0.00 O |
| ATOM | 1465 H | GLY A 100122.518 | -6.644 | 20.714 | 1.00 | 0.00 H |
| ATOM | 1466 1HA | GLY A 100121.420 | -4.864 | 18.779 | 1.00 | 0.00 H |
| ATOM | 1467 2HA | GLY A 100120.537 | -6.085 | 19.685 | 1.00 | 0.00 H |
| ATOM | 1468 N | PRO A 101120.221 | -4.486 | 21.866 | 1.00 | 0.00 N |
| ATOM | 1469 CA | PRO A 101119.600 | -3.515 | 22.773 | 1.00 | 0.00 C |
| ATOM | 1470 C | PRO A 101120.582 | -2.443 | 23.233 | 1.00 | 0.00 C |
| ATOM | 1471 O | PRO A 101121.475 | -2.709 | 24.038 | 1.00 | 0.00 O |
| ATOM | 1472 CB | PRO A 101119.150 | -4.372 | 23.959 | 1.00 | 0.00 C |
| ATOM | 1473 CG | PRO A 101120.062 | -5.549 | 23.942 | 1.00 | 0.00 C |
| ATOM | 1474 CD | PRO A 101120.374 | -5.812 | 22.495 | 1.00 | 0.00 C |
| ATOM | 1475 HA | PRO A 101118.741 | -3.043 | 22.319 | 1.00 | 0.00 H |
| ATOM | 1476 1HB | PRO A 101119.249 | -3.806 | 24.873 | 1.00 | 0.00 H |
| ATOM | 1477 2HB | PRO A 101118.121 | -4.669 | 23.821 | 1.00 | 0.00 H |
| ATOM | 1478 1HG | PRO A 101120.966 | -5.320 | 24.485 | 1.00 | 0.00 H |
| ATOM | 1479 2HG | PRO A 101119.566 | -6.403 | 24.379 | 1.00 | 0.00 H |
| ATOM | 1480 1HD | PRO A 101121.386 | -6.175 | 22.387 | 1.00 | 0.00 H |
| ATOM | 1481 2HD | PRO A 101119.671 | -6.518 | 22.079 | 1.00 | 0.00 H |
| ATOM | 1482 N | SER A 102120.410 | -1.230 | 22.718 | 1.00 | 0.00 N |
| ATOM | 1483 CA | SER A 102121.282 | -0.117 | 23.077 | 1.00 | 0.00 C |
| ATOM | 1484 C | SER A 102120.786 | 0.576 | 24.341 | 1.00 | 0.00 C |
| ATOM | 1485 O | SER A 102121.581 | 1.051 | 25.153 | -1.00 | 0.00 O |

1.00 0.00 C SER A 102121.358 0.889 21.926 **ATOM** 1486 CB SER A 102120.064 1.307 21.527 1.00 0.00 O **ATOM** 1487 OG 0.00 H SER A 102119.679 -1.080 22.081 1.00 **ATOM** 1488 Η SER A 102122.268 -0.515 23.261 1.00 0.00 H **ATOM** 1489 HA**ATOM** 1490 1HB SER A 102121.918 1.755 22.245 1.00 0.00 H 1.00 0.00 H SER A 102121.851 0.430 21.082 **ATOM** 1491 2HB 0.00 H SER A 102119.966 2.248 21.690 1.00 **ATOM** 1492 HG 0.00 N 1.00 **ATOM** 1493 N SER A 103119.468 0.630 24.503 0.00 C 1.00 SER A 103118.867 1.265 25.670 **ATOM** 1494 CA \mathbf{C} SER A 103119.270 0.543 26.952 1.00 0.00 C **ATOM** 1495 0.00 O -0.550 27.240 1.00 **ATOM** 1496 O SER A 103118.782 0.00 C 1.283 25.539 1.00 SER A 103117.343 **ATOM** 1497 CB 0.00 O 1498 OG SER A 103116.799 2.484 26.058 1.00 **ATOM** 1.00 0.00 H 23.821 1499 H SER A 103118.886 0.234 **ATOM** 2.282 25.716 1.00 0.00 H **ATOM** 1500 HA SER A 103119.226 SER A 103117.073 1.202 24.497 1.00 0.00 H**ATOM** 1501 1HB 26.083 1.00 0.00 H SER A 103116.927 0.448 **ATOM** 1502 2HB SER A 103116.312 2.293 26.864 1.00 0.00 H **ATOM** 1503 HG 1.00 0.00 N 27.717 GLY A 104120.165 1.160 **ATOM** 1504 N 28.957 1.00 0.00 C 1505 GLY A 104120.618 0.561 **ATOM** CA 0.545 30.022 1.00 0.00 C **ATOM** 1506 \mathbf{C} GLY A 104119.539 0.00 O 31.070 1.00 1507 0 GLY A 104119.748 -0.103 **ATOM** 0.00 O OXT GLY A 104118.485 1.179 29.809 1.00 **ATOM** 1508 1.00 0.00 H2.029 27.436 GLY A 104120.520 **ATOM** 1509 H 28.762 1.00 0.00 H 1510 1HA GLY A 104120.930 -0.455 **ATOM** 0.00 H 1511 2HA GLY A 104121.464 29.327 1.00 1.121 **ATOM** 1512 GLY A 104 **TER**

ENDMDL

| ATOM 1 | N | GLY A | 1105.215 | 7.354 | -0.195 | 1.00 | 0.00 N |
|-----------|----|-------|----------|-------|--------|------|--------|
| ATOM 2 | CA | GLY A | 1106.288 | 6.361 | -0.481 | 1.00 | 0.00 C |
| ATOM 3 | С | GLY A | 1107.290 | 6.250 | 0.651 | 1.00 | 0.00 C |
| ATOM 4 | С | GLY A | 1107.077 | 6.795 | 1.734 | 1.00 | 0.00 O |
| ATOM 5 1H | ł | GLY A | 1105.533 | 8.026 | 0.533 | 1.00 | 0.00 H |
| ATOM 6 2H | ł | GLY A | 1104.360 | 6.869 | 0.147 | 1.00 | 0.00 H |
| ATOM 7 3H | ł | GLY A | 1104.976 | 7.882 | -1.060 | 1.00 | 0.00 H |
| ATOM 8 1H | łΑ | GLY A | 1105.834 | 5.395 | -0.642 | 1.00 | 0.00 H |
| ATOM 9 2H | ΙA | GLY A | 1106.807 | 6.659 | -1.380 | 1.00 | 0.00 H |
| ATOM10 | N | SER A | 2108.386 | 5.542 | 0.400 | 1.00 | 0.00 N |
| ATOM11 | CA | SER A | 2109.426 | 5.360 | 1.405 | 1.00 | 0.00 C |
| ATOM12 | C | SER A | 2110.256 | 6.629 | 1.565 | 1.00 | 0.00 C |
| ATOM13 | O | SER A | 2110.259 | 7.496 | 0.691 | 1.00 | 0.00 O |
| ATOM14 | СВ | SER A | 2110.332 | 4.187 | 1.026 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2109.867 | 2.977 | 1.597 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2108.498 | 5.132 | -0.484 | 1.00 | 0.00 H |
| ATOM17 | HA | SER A | 2108.942 | 5.140 | 2.346 | 1.00 | 0.00 H |
| ATOM18 11 | НВ | SER A | 2110.348 | 4.080 | -0.048 | 1.00 | 0.00 H |
| ATOM19 21 | НВ | SER A | 2111.334 | 4.379 | 1.384 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2110.095 | 2.955 | 2.530 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3110.962 | 6.731 | 2.687 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3111.797 | 7.894 | 2.960 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3113.078 | 7.853 | 2.131 | 1.00 | 0.00 C |
| ATOM24 | О | SER A | 3113.500 | 8.866 | 1.573 | 1.00 | 0.00 O |

| ATOM25 | СВ | SER A | 3112.142 | 7.961 | 4.450 | 1.00 | 0.00 C |
|----------|-----|-------|----------|-------|-------|------|--------|
| ATOM26 | OG | SER A | 3113.199 | 7.072 | 4.769 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3110.920 | 6.008 | 3.346 | 1.00 | 0.00 H |
| ATOM28 | НА | SER A | 3111.237 | 8.777 | 2.690 | 1.00 | 0.00 H |
| ATOM29 1 | НВ | SER A | 3112.447 | 8.967 | 4.702 | 1.00 | 0.00 H |
| ATOM30 2 | HB | SER A | 3111.272 | 7.692 | 5.031 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3112.849 | 6.184 | 4.872 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4113.690 | 6.676 | 2.056 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4114.915 | 6.525 | 1.294 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4116.155 | 6.661 | 2.156 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4116.173 | 7.435 | 3.112 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4113.307 | 5.904 | 2.523 | 1.00 | 0.00 H |
| ATOM37 | НА | GLY A | 4114.918 | 5.550 | 0.828 | 1.00 | 0.00 H |
| ATOM38 2 | 2HA | GLY A | 4114.941 | 7.280 | 0.523 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5117.194 | 5.905 | 1.817 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5118.444 | 5.943 | 2.567 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5119.548 | 5.197 | 1.823 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5119.739 | 3.997 | 2.018 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5118.248 | 5.336 | 3.957 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5117.949 | 3.954 | 3.871 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5117.119 | 5.306 | 1.044 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5118.734 | 6.978 | 2.673 | 1.00 | 0.00 H |
| ATOM47 | lНВ | SER A | 5119.154 | 5.461 | 4.533 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5117.433 | 5.839 | 4.455 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5117.186 | 3.826 | 3.304 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6120.271 | 5.917 | 0.971 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6121.355 | 5.322 | 0.198 | 1.00 | 0.00 C |

| ATOM52 | C | SER A | 6122.687 | 5.469 | 0.929 | 1.00 | 0.00 C |
|--------|-----|-------|----------|--------|--------|------|--------|
| ATOM53 | O | SER A | 6123.365 | 6.489 | 0.805 | 1.00 | 0.00 O |
| ATOM54 | CB | SER A | 6121.443 | 5.975 | -1.182 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6120.178 | 5.990 | -1.821 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6120.070 | 6.869 | 0.859 | 1.00 | 0.00 H |
| ATOM57 | HA | SER A | 6121.140 | 4.271 | 0.077 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6121.790 | 6.992 | -1.076 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6122.137 | 5.420 | -1.796 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6119.653 | 6.716 | -1.475 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7123.055 | 4.444 | 1.688 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7124.304 | 4.477 | 2.428 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7125.284 | 3.418 | 1.960 | 1.00 | 0.00 C |
| ATOM64 | Ο | GLY A | 7126.040 | 2.867 | 2.760 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7122.474 | 3.656 | 1.750 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7124.757 | 5.450 | 2.304 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7124.095 | 4.321 | 3.475 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8125.269 | 3.134 | 0.662 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8126.163 | 2.134 | 0.089 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8127.308 | 2.798 | -0.668 | 1.00 | 0.00 C |
| ATOM71 | О | LEU A | 8128.424 | 2.279 | -0.705 | 1.00 | 0.00 O |
| ATOM72 | CB | LEU A | 8125.389 | 1.205 | -0.847 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8124.503 | 0.173 | -0.148 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8123.307 | -0.182 | -1.018 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8125.306 | -1.075 | 0.192 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8124.644 | 3.608 | 0.076 | 1.00 | 0.00 H |
| ATOM77 | НА | LEU A | 8126.573 | 1.553 | 0.901 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8124.763 | 1.811 | -1.486 | 1.00 | 0.00 H |

0.676 -1.465 8126.099 1.00 0.00 H ATOM79 2HB LEU A 0.775 1.00 0.00 H ATOM80 HG LEUA 8124.130 0.594 -0.390 1.00 0.00 H ATOM81 1HD1 LEU A 8122.467 -0.437 -1.026 -1.646 1.00 0.00 H ATOM82 2HD1 LEU A 8123.557 ATOM83 3HD1 LEU A 8123.050 0.664 -1.638 1.00 0.00 H 8124.669 -1.943 0.118 1.00 0.00 H ATOM84 1HD2 LEU A 8125.689 -0.992 1.198 1.00 0.00 H ATOM85 2HD2 LEU A ATOM86 3HD2 LEU A 8126.129 -1.171 -0.500 1.00 0.00 H 9127.025 -1.271 1.00 0.00 N ATOM87 N 3.949 **ALAA** 9128.032 -2.027 1.00 0.00 C ATOM88 CA ALA A 4.684 ATOM89 C **ALAA** 9128.353 6.018 -1.362 1.00 0.00 C 6.685 -0.828 1.00 0.00 O 9127.467 ATOM90 О ALAA 9127.559 4.904 -3.456 1.00 0.00 C ATOM91 CB ALA A 4.312 -1.204 0.00 H 9126.117 1.00 ATOM92 Η **ALAA** -2.058 1.00 0.00 H 9128.930 4.083 ATOM93 HA ALAA -3.766 0.00 H ATOM94 1HB ALA A 9126.948 4.070 1.00 9128.415 -4.110 1.00 0.00 HATOM95 2HB ALA A 4.986 -3.507 1.00 0.00 HATOM96 3HB 9126.979 5.813 ALA A 1.00 0.00 N ATOM97 N -1.399 MET A 10129.625 6.399 -0.799 1.00 0.00 C MET A 10130.064 7.654 ATOM98 CA 0.00 C ATOM99 \mathbf{C} MET A 10131.140 8.320 -1.656 1.00 MET A 10132.329 8.052 -1.490 1.00 0.00 O **ATOM** 100 0 0.612 1.00 0.00 C **ATOM** 101 CB**MET A** 10130.601 7.410 1.00 0.00 C 1.634 **ATOM** 102 CG **MET A** 10129.515 7.117 2.905 1.00 0.00 S MET A 10130.052 5.956 **ATOM** 103 SD 1.00 0.00 C 10128.479 5.283 3.435 **ATOM** 104 CE **MET A** 1.00 0.00 H -1.839 MET A 10130.285 5.823 **ATOM** 105 Η

| ATOM | 106 | НА | MET A | 10129.209 | 8.311 | -0.740 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 107 1 | НВ | MET A | 10131.277 | 6.568 | 0.586 | 1.00 | 0.00 H |
| ATOM | 108 2 | 2HB | MET A | 10131.144 | 8.286 | 0.935 | 1.00 | 0.00 H |
| ATOM | 109 1 | HG | MET A | 10129.229 | 8.043 | 2.110 | 1.00 | 0.00 H |
| ATOM | 110 2 | HG | MET A | 10128.661 | 6.699 | 1.121 | 1.00 | 0.00 H |
| ATOM | 111 1 | HE | MET A | 10127.696 | 6.001 | 3.239 | 1.00 | 0.00 H |
| ATOM | 112 2 | HE | MET A | 10128.516 | 5.071 | 4.493 | 1.00 | 0.00 H |
| ATOM | 113 3 | HE | MET A | 10128.277 | 4.371 | 2.892 | 1.00 | 0.00 H |
| ATOM | 114 | N | PRO A | 11130.733 | 9.201 | -2.588 | 1.00 | 0.00 N |
| ATOM | 115 | CA | PRO A | 11131.672 | 9.903 | -3.467 | 1.00 | 0.00 C |
| ATOM | 116 | C | PRO A | 11132.708 | 10.710 | -2.687 | 1.00 | 0.00 C |
| ATOM | 117 | О | PRO A | 11133.901 | 10.639 | -2.976 | 1.00 | 0.00 O |
| ATOM | 118 | СВ | PRO A | 11130.781 | 10.836 | -4.295 | 1.00 | 0.00 C |
| ATOM | 119 | CG | PRO A | 11129.406 | 10.270 | -4.185 | 1.00 | 0.00 C |
| ATOM | 120 | CD | PRO A | 11129.335 | 9.581 | -2.851 | 1.00 | 0.00 C |
| ATOM | 121 | НА | PRO A | 11132.181 | 9.214 | -4.125 | 1.00 | 0.00 H |
| ATOM | 122 | lНВ | PRO A | 11130.831 | 11.836 | -3.892 | 1.00 | 0.00 H |
| ATOM | 123 2 | 2НВ | PRO A | 11131.120 | 10.841 | -5.321 | 1.00 | 0.00 H |
| ATOM | 124 | HG | PRO A | 11128.680 | 11.066 | -4.229 | 1.00 | 0.00 H |
| ATOM | 125 2 | 2HG | PRO A | 11129.236 | 9.561 | -4.981 | 1.00 | 0.00 H |
| ATOM | 126 | IHD | PRO A | 11128.971 | 10.260 | -2.095 | 1.00 | 0.00 H |
| ATOM | 127 2 | 2HD | PRO A | 11128.704 | 8.707 | -2.911 | 1.00 | 0.00 H |
| ATOM | 128 | N | PRO A | 12132.269 | 11.487 | -1.678 | 1.00 | 0.00 N |
| ATOM | 129 | CA | PRO A | 12133.179 | 12.297 | -0.861 | 1.00 | 0.00 C |
| ATOM | 130 | C | PRO A | 12134.284 | 11.455 | -0.232 | 1.00 | 0.00 C |
| ATOM | 131 | О | PRO A | 12135.340 | 11.970 | 0.133 | 1.00 | 0.00 O |
| ATOM | 132 | СВ | PRO A | 12132.272 | 12.882 | 0.225 | 1.00 | 0.00 C |

| ATOM | 133 | CG | PRO A | 12130.903 | 12.847 | -0.360 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 134 | CD | PRO A | 12130.866 | 11.636 | -1.249 | 1.00 | 0.00 C |
| ATOM | 135 | НА | PRO A | 12133.622 | 13.096 | -1.437 | 1.00 | 0.00 H |
| ATOM | 136 1 | НВ | PRO A | 12132.336 | 12.276 | 1.117 | 1.00 | 0.00 H |
| ATOM | 137 2 | НВ | PRO A | 12132.579 | 13.893 | 0.447 | 1.00 | 0.00 H |
| ATOM | 138 1 | HG | PRO A | 12130.170 | 12.758 | 0.426 | 1.00 | 0.00 H |
| ATOM | 139 2 | HG | PRO A | 12130.728 | 13.741 | -0.940 | 1.00 | 0.00 H |
| ATOM | 140 1 | HD | PRO A | 12130.539 | 10.770 | -0.691 | 1.00 | 0.00 H |
| ATOM | 141 2 | HD | PRO A | 12130.219 | 11.809 | -2.094 | 1.00 | 0.00 H |
| ATOM | 142 | N | GLY A | 13134.030 | 10.155 | -0.108 | 1.00 | 0.00 N |
| ATOM | 143 | CA | GLY A | 13135.012 | 9.261 | 0.477 | 1.00 | 0.00 C |
| ATOM | 144 | C | GLY A | 13135.208 | 7.999 | -0.339 | 1.00 | 0.00 C |
| ATOM | 145 | О | GLY A | 13135.145 | 6.891 | 0.193 | 1.00 | 0.00 O |
| ATOM | 146 | Н | GLY A | 13133.170 | 9.800 | -0.417 | 1.00 | 0.00 H |
| ATOM | 147 1 | НА | GLY A | 13135.957 | 9.779 | 0.552 | 1.00 | 0.00 H |
| ATOM | 148 2 | HA | GLY A | 13134.686 | 8.986 | 1.470 | 1.00 | 0.00 H |
| ATOM | 149 | N | ASN A | 14135.447 | 8.169 | -1.638 | 1.00 | 0.00 N |
| ATOM | 150 | CA | ASN A | 14135.654 | 7.038 | -2.536 | 1.00 | 0.00 C |
| ATOM | 151 | C | ASN A | 14134.405 | 6.163 | -2.612 | 1.00 | 0.00 C |
| ATOM | 152 | О | ASN A | 14133.628 | 6.256 | -3.562 | 1.00 | 0.00 O |
| ATOM | 153 | СВ | ASN A | 14136.854 | 6.205 | -2.078 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14138.169 | 6.936 | -2.265 | 1.00 | 0.00 C |
| ATOM | 155 | ODI | ASN A | 14138.694 | 7.023 | -3.375 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14138.711 | 7.466 | -1.173 | 1.00 | 0.00 N |
| ATOM | 157 | Н | ASN A | 14135.485 | 9.078 | -2.000 | 1.00 | 0.00 H |
| ATOM | 158 | НА | ASN A | 14135.858 | 7.433 | -3.520 | 1.00 | 0.00 H |
| ATOM | 159 1 | НВ | ASN A | 14136.742 | 5.965 | -1.032 | 1.00 | 0.00 H |

| ATOM | 160 2 | 2HB | ASN A | 14136.888 | 5.290 | -2.652 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|-------|--------|------|---------|
| ATOM | 161 1 | HD2 | ASN A | 14138.237 | 7.357 | -0.322 | 1.00 | 0.00 H |
| ATOM | 162 2 | 2HD2 | ASN A | 14139.561 | 7.945 | -1.264 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15134.219 | 5.312 | -1.607 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15133.065 | 4.422 | -1.564 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15132.542 | 4.276 | -0.139 | 1.00 | 0.00 C |
| ATOM | 166 | О | SER A | 15131.340 | 4.379 | 0.107 | 1.00 | 0.00 O |
| ATOM | 167 | CB | SER A | 15133.432 | 3.048 | -2.127 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15132.293 | 2.391 | -2.653 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15134.872 | 5.282 | -0.878 | 1.00 | 0.00 H |
| ATOM | 170 | HA | SER A | 15132.289 | 4.856 | -2.176 | 1.00 | 0.00 H |
| ATOM | 171 1 | lНВ | SER A | 15134.159 | 3.167 | -2.917 | 1.00 | 0.00 H |
| ATOM | 172 2 | 2HB | SER A | 15133.853 | 2.439 | -1.340 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15131.783 | 3.007 | -3.183 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16133.453 | 4.036 | 0.799 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.084 | 3.876 | 2.201 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16133.923 | 4.787 | 3.092 | 1.00 | 0.00 C |
| ATOM | 177 | О | HIS A | 16133.400 | 5.454 | 3.984 | 1.00 | 0.00 O |
| ATOM | 178 | СВ | HIS A | 16133.259 | 2.420 | 2.633 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16132.025 | 1.591 | 2.457 | 1.00 | 0.00 C. |
| ATOM | 180 | ND1 | HIS A | 16131.474 | 0.835 | 3.472 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16131.232 | 1.401 | 1.377 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16130.397 | 0.216 | 3.023 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16130.227 | 0.543 | 1.755 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16134.396 | 3.965 | 0.542 | 1.00 | 0.00 H |
| ATOM | 185 | НА | HIS A | 16132.045 | 4.150 | 2.304 | 1.00 | 0.00 H |
| ATOM | 186 | 1HB | HIS A | 16134.047 | 1.970 | 2.047 | 1.00 | 0.00 H |

| ATOM | 187 | 2HB | HIS A | 16133.534 | 2.391 | 3.678 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 188 | HD1 | HIS A | 16131.822 | 0.763 | 4.385 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16131.363 | 1.841 | 0.399 | 1.00 | 0.00 H |
| ATOM | 190 | HE1 | HIS A | 16129.763 | -0.444 | 3.596 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16129.457 | 0.291 | 1.205 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.229 | 4.809 | 2.843 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17136.120 | 5.641 | 3.630 | 1.00 | 0.00 C |
| ATOM | 194 | C | GLY A | 17137.532 | 5.092 | 3.679 | 1.00 | 0.00 C |
| ATOM | 195 | О | GLY A | 17138.032 | 4.742 | 4.748 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.589 | 4.257 | 2.119 | 1.00 | 0.00 H |
| ATOM | 197 | 1HA | GLY A | 17136.145 | 6.631 | 3.200 | 1.00 | 0.00 H |
| ATOM | 198 | 2HA | GLY A | 17135.736 | 5.707 | 4.637 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18138.175 | 5.015 | 2.519 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.539 | 4.503 | 2.434 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.547 | 5.574 | 2.836 | 1.00 | 0.00 C |
| ATOM | 202 | О | LEU A | 18140.918 | 6.426 | 2.029 | 1.00 | 0.00 O |
| ATOM | 203 | CB | LEU A | 18139.833 | 4.014 | 1.015 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18138.730 | 3.165 | 0.380 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18138.853 | 3.178 | -1.136 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18138.786 | 1.740 | 0.909 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.723 | 5.308 | 1.701 | 1.00 | 0.00 H |
| ATOM | 208 | HA | LEU A | 18139.623 | 3.672 | 3.116 | 1.00 | 0.00 H |
| ATOM | 209 | 1HB | LEU A | 18140.002 | 4.877 | 0.387 | 1.00 | 0.00 H |
| ATOM | 210 | 2HB | LEU A | 18140.739 | 3.426 | 1.040 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18137.769 | 3.583 | 0.641 | 1.00 | 0.00 H |
| ATOM | 212 | 1HD1 | LEU A | 18139.875 | 2.973 | -1.416 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18138.564 | 4.149 | -1.512 | 1.00 | 0.00 H |

| ATOM | 214 3 | BHD1 | LEU A | 18138.205 | 2.423 | -1.556 | 1.00 | 0.00 H |
|------|-------|---------------------------|-------|-----------|-------|--------|------|--------|
| ATOM | 215 | HD2 | LEU A | 18137.874 | 1.224 | 0.648 | 1.00 | 0.00 H |
| ATOM | 216 2 | 2HD2 | LEU A | 18138.895 | 1.758 | 1.983 | 1.00 | 0.00 H |
| ATOM | 2173 | 3HD2 | LEU A | 18139.629 | 1.226 | 0.470 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19140.988 | 5.523 | 4.088 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.956 | 6.488 | 4.598 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19143.006 | 5.799 | 5.464 | 1.00 | 0.00 C |
| ATOM | 221 | О | GLU A | 19142.962 | 4.585 | 5.662 | 1.00 | 0.00 O |
| ATOM | 222 | СВ | GLU A | 19141.246 | 7.576 | 5.405 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.290 | 7.030 | 6.453 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19140.046 | 8.008 | 7.586 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19139.639 | 7.561 | 8.679 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19140.261 | 9.220 | 7.380 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.656 | 4.819 | 4.684 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.447 | 6.944 | 3.751 | 1.00 | 0.00 H |
| ATOM | 229 | lНВ | GLU A | 19141.989 | 8.180 | 5.907 | 1.00 | 0.00 H |
| ATOM | 230 2 | 2HB | GLU A | 19140.683 | 8.202 | 4.728 | 1.00 | 0.00 H |
| ATOM | 231 | lHG | GLU A | 19139.345 | 6.807 | 5.981 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19140.708 | 6.122 | 6.864 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.949 | 6.582 | 5.978 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL A | 20145.009 | 6.047 | 6.822 | 1.00 | 0.00 C |
| ATOM | 235 | $\mathbf{C}_{\mathbf{q}}$ | VAL A | 20144.435 | 5.407 | 8.082 | 1.00 | 0.00 C |
| ATOM | 236 | О | VAL A | 20143.542 | 5.963 | 8.722 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20146.013 | 7.144 | 7.229 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20147.191 | 6.540 | 7.979 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VAL A | 20146.489 | 7.914 | 6.004 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.931 | 7.543 | 5.783 | 1.00 | 0.00 H |

| . = ~ | | | **** | 00145 500 | 5 204 | ()57 | 1.00 | 0.00 11 |
|-------|-----|------|-------|-----------|--------|--------|------|---------|
| ATOM | 241 | HA | VAL A | 20145.539 | 5.294 | 6.257 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.512 | 7.835 | 7.889 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20147.488 | 5.618 | 7.501 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20146.903 | 6.341 | 9.000 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20148.019 | 7.235 | 7.967 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20147.486 | 7.592 | 5.743 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20146.498 | 8.971 | 6.226 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20145.821 | 7.726 | 5.177 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.954 | 4.234 | 8.432 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.482 | 3.538 | 9.615 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.450 | 2.476 | 9.287 | 1.00 | 0.00 C |
| ATOM | 252 | О | GLY A | 21143.375 | 1.447 | 9.959 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.665 | 3.840 | 7.885 | 1.00 | 0.00 H |
| ATOM | 254 | 1HA | GLY A | 21145.323 | 3.069 | 10.104 | 1.00 | 0.00 H |
| ATOM | 255 | 2HA | GLY A | 21144.039 | 4.256 | 10.290 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.655 | 2.725 | 8.253 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.623 | 1.781 | 7.837 | 1.00 | 0.00 C |
| ATOM | 258 | С | SER A | 22142.196 | 0.728 | 6.895 | 1.00 | 0.00 C |
| ATOM | 259 | O | SER A | 22143.138 | 0.996 | 6.147 | 1.00 | 0.00 O |
| ATOM | 260 | СВ | SER A | 22140.471 | 2.521 | 7.154 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22140.308 | 3.821 | 7.694 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.764 | 3.562 | 7.756 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22141.249 | 1.289 | 8.722 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.678 | 2.607 | 6.098 | 1.00 | 0.00 H |
| ATOM | 265 | 2HB | SER A | 22139.556 | 1.967 | 7.298 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22140.349 | 3.777 | 8.653 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.624 | -0.470 | 6.936 | 1.00 | 0.00 N |
| | | | | | | | | |

| ATOM | 268 | CA | LEU A | 23142.078 | -1.564 | 6.086 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 269 | C | LEU A | 23141.426 | -1.492 | 4.709 | 1.00 | 0.00 C |
| ATOM | 270 | O | LEU A | 23140.229 | -1.231 | 4.590 | 1.00 | 0.00 O |
| ATOM | 271 | СВ | LEU A | 23141.763 | -2.911 | 6.740 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23142.577 | -3.225 | 7.997 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23141.779 | -4.108 | 8.943 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.893 | -3.892 | 7.624 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.877 | -0.622 | 7.552 | 1.00 | 0.00 H |
| ATOM | 276 | НА | LEU A | 23143.148 | -1.472 | 5.970 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.716 | -2.923 | 7.003 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.945 | -3.691 | 6.017 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.803 | -2.303 | 8.512 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23141.062 | -4.686 | 8.378 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23141.259 | -3.490 | 9.659 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23142.449 | -4.777 | 9.464 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23143.706 | -4.908 | 7.309 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23144.550 | -3.897 | 8.481 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23144.359 | -3.345 | 6.818 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.222 | -1.725 | 3.670 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.724 | -1.686 | 2.301 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALAA | 24142.324 | -2.812 | 1.466 | 1.00 | 0.00 C |
| ATOM | 289 | Ο | ALA A | 24143.420 | -3.294 | 1.751 | 1.00 | 0.00 O |
| ATOM | 290 | СВ | ALA A | 24142.028 | -0.337 | 1.667 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24143.168 | -1.928 | 3.829 | 1.00 | 0.00 H |
| ATOM | 292 | НА | ALA A | 24140.651 | -1.808 | 2.334 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALA A | 24141.196 | 0.333 | 1.830 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24142.184 | -0.464 | 0.606 | 1.00 | 0.00 H |

| ATOM | 295 3 | НВ | ALA A | 24142.919 | 0.079 | 2.115 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|---------|------|--------|
| ATOM | 296 | N | GLU A | 25141.598 | -3.227 | 0.433 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.059 | -4.299 | -0.445 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.225 | -3.797 | -1.876 | 1.00 | 0.00 C |
| ATOM | 299 | O | GLU A | 25141.447 | -2.968 | -2.348 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25141.075 | -5.470 | -0.414 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.514 | -6.654 | -1.260 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.767 | -6.737 | -2.578 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25140.490 | -5.674 | -3.170 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25140.461 | -7.865 | -3.017 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25140.732 | -2.805 | 0.256 | 1.00 | 0.00 H |
| ATOM | 306 | НА | GLU A | 25143.017 | -4.636 | -0.081 | 1.00 | 0.00 H |
| ATOM | 307 1 | НВ | GLU A | 25140.965 | -5.805 | 0.607 | 1.00 | 0.00 H |
| ATOM | 308 2 | 2HB | GLU A | 25140.117 | -5.130 | -0.778 | 1.00 | 0.00 H |
| ATOM | 309 1 | HG | GLU A | 25142.569 | -6.561 | -1.469 | 1.00 | 0.00 H |
| ATOM | 310 2 | 2HG | GLU A | 25141.335 | -7.563 | -0.704 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.244 | -4.305 | -2.560 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VALA | 26143.513 | -3.909 | -3.937 | 1.00 | 0.00 C |
| ATOM | 313 | C | VAL A | 26142.949 | -4.926 | -4.922 | 1.00 | 0.00 C |
| ATOM | 314 | O | VAL A | 26142.719 | -6.084 | -4.571 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VALA | 26145.024 | -3.751 | -4.191 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VAL A | 26145.275 | -3.136 | -5.559 | 1.00 | 0.00 C |
| ATOM | 317 | CG2 | VALA | 26145.665 | -2.911 | -3.097 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.830 | -4.962 | - 2.129 | 1.00 | 0.00 H |
| ATOM | 319 | НА | VAL A | 26143.039 | -2.953 | -4.109 | 1.00 | 0.00 H |
| ATOM | 320 | НВ | VAL A | 26145.477 | -4.731 | -4.173 | 1.00 | 0.00 H |
| ATOM | 321 | IHG1 | VAL A | 26146.222 | -2.616 | -5.553 | 1.00 | 0.00 H |

| ATOM | 322 2HG | 1 VAL A | 26144.484 | - 2.439 | -5.792 | 1.00 | 0.00 H |
|-------|---------|---------|-----------|---------|--------|------|--------|
| ATOM | 323 3HG | 1 VAL A | 26145.299 | -3.917 | -6.305 | 1.00 | 0.00 H |
| ATOM | 324 1HG | 2 VAL A | 26145.381 | -1.876 | -3.223 | 1.00 | 0.00 H |
| ATOM | 325 2HG | 2 VAL A | 26146.740 | -2.998 | -3.157 | 1.00 | 0.00 H |
| ATOM | 326 3HG | 2 VALA | 26145.330 | -3.260 | -2.131 | 1.00 | 0.00 H |
| ATOM | 327 N | LYS A | 27142.727 | -4.487 | -6.157 | 1.00 | 0.00 N |
| ATOM | 328 CA | LYS A | 27142.188 | -5.360 | -7.194 | 1.00 | 0.00 C |
| ATOM | 329 C | LYS A | 27143.310 | -5.966 | -8.031 | 1.00 | 0.00 C |
| ATOM | 330 O | LYS A | 27143.259 | -5.951 | -9.262 | 1.00 | 0.00 O |
| ATOM | 331 CB | LYS A | 27141.223 | -4.583 | -8.092 | 1.00 | 0.00 C |
| ATOM | 332 CG | LYSA | 27139.924 | -4.202 | -7.403 | 1.00 | 0.00 C |
| ATOM | 333 CD | LYSA | 27139.048 | -5.419 | -7.154 | 1.00 | 0.00 C |
| 'ATOM | 334 CE | LYS A | 27137.646 | -5.018 | -6.724 | 1.00 | 0.00 C |
| ATOM | 335 NZ | LYSA | 27137.102 | -5.932 | -5.682 | 1.00 | 0.00 N |
| ATOM | 336 H | LYS A | 27142.930 | -3.554 | -6.376 | 1.00 | 0.00 H |
| ATOM | 337 HA | LYSA | 27141.648 | -6.158 | -6.706 | 1.00 | 0.00 H |
| ATOM | 338 1HB | LYS A | 27141.710 | -3.677 | -8.424 | 1.00 | 0.00 H |
| ATOM | 339 2HB | LYS A | 27140.985 | -5.190 | -8.954 | 1.00 | 0.00 H |
| ATOM | 340 1HG | LYS A | 27140.152 | -3.735 | -6.457 | 1.00 | 0.00 H |
| ATOM | 341 2HG | LYS A | 27139.387 | -3.504 | -8.030 | 1.00 | 0.00 H |
| ATOM | 342 1HD | LYS A | 27138.983 | -5.995 | -8.065 | 1.00 | 0.00 H |
| ATOM | 343 2HD | LYS A | 27139.496 | -6.019 | -6.376 | 1.00 | 0.00 H |
| ATOM | 344 1HE | LYS A | 27137.678 | -4.014 | -6.327 | 1.00 | 0.00 H |
| ATOM | 345 2HE | LYS A | 27136.998 | -5.043 | -7.587 | 1.00 | 0.00 H |
| ATOM | 346 1HZ | LYS A | 27136.733 | -6.799 | -6.124 | 1.00 | 0.00 H |
| ATOM | 347 2HZ | LYS A | 27136.331 | -5.466 | -5.163 | 1.00 | 0.00 H |
| ATOM | 348 3HZ | LYS A | 27137.851 | -6.192 | -5.007 | 1.00 | 0.00 H |

| ATOM | 349 | N | GLU A | 28144.323 | -6.501 | -7.357 | 1.00 | 0.00 N |
|------|-------|-----|-------|-------------|-----------|--------|------|--------|
| ATOM | 350 | CA | GLU A | 28145.457 | -7.112 | -8.038 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.269 | -8.622 | -8.160 | 1.00 | 0.00 C |
| AŢOM | 352 | O | GLU A | 28144.303 | -9.181 | -7.640 | 1.00 | 0.00 O |
| ATOM | 353 | СВ | GLU A | 28146.756 | -6.806 | -7.288 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28147.863 | -6.272 | -8.182 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28149.224 | -6.837 | -7.824 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28149.635 | -7.835 | -8.452 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28149.878 | -6.281 | -6.917 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.307 | -6.483 | -6.377 | 1.00 | 0.00 H |
| ATOM | 359 | НА | GLU A | 28145.516 | -6.688 | -9.029 | 1.00 | 0.00 H |
| ATOM | 360 1 | IHB | GLU A | 28146.552 | -6.068 | -6.526 | 1.00 | 0.00 H |
| ATOM | 361 2 | 2HB | GLU A | 28147.110 | -7.711 | -6.814 | 1.00 | 0.00 H |
| ATOM | 362 | IHG | GLU A | 28147.640 | -6.533 | -9.205 | 1.00 | 0.00 H |
| ATOM | 363 2 | 2HG | GLU A | 28147.899 | -5.197 | -8.085 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29146.199 | -9.275 | -8.850 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29146.136 - | -10.719 | -9.040 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29146:156 - | 11.446 | -7.697 | 1.00 | 0.00 C |
| ATOM | 367 | O | ASN A | 29145.239 - | 12.204 | -7.381 | 1.00 | 0.00 O |
| ATOM | 368 | CB | ASN A | 29147.306 | -11.191 | -9.907 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29146.930 | -11.306 - | 11.371 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29146.786 - | 12.407 - | 11.903 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29146.767 - | 10.165 - | 12.032 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29146.944 | -8.773 | -9.240 | 1.00 | 0.00 H |
| ATOM | 373 | HA | ASN A | 29145.211 | -10.947 | -9.546 | 1.00 | 0.00 H |
| ATOM | 374 | 1HB | ASN A | 29148.119 - | 10.486 | -9.819 | 1.00 | 0.00 H |
| ATOM | 375 | 2HB | ASN A | 29147.635 - | 12.160 | -9.561 | 1.00 | 0.00 H |

| ATOM | 376 1HD2 ASN A | 29146.898 -9.325 - | 1.543 1.0 | 0.00 H |
|------|----------------|----------------------|------------|------------|
| ATOM | 377 2HD2 ASN A | 29146.524 -10.210 -1 | 2.979 1.00 | O.00 H |
| ATOM | 378 N PRO A | 30147.206 -11.226 | -6.887 1.0 | 00 0.00 N |
| ATOM | 379 CA PRO A | 30147.337 -11.863 | -5.575 1. | 00 0.00 C |
| ATOM | 380 C PRO A | 30146.420 -11.233 | -4.529 1.0 | 00 0.00 C |
| ATOM | 381 O PRO A | 30146.641 -10.098 | -4.105 1.0 | O 0.00 O |
| ATOM | 382 CB PROA | 30148.802 -11.621 | -5.217 1. | 00 0.00 C |
| ATOM | 383 CG PROA | 30149.156 -10.354 | -5.917 1. | 00 0.00 C |
| ATOM | 384 CD PROA | 30148.346 -10.336 | -7.187 1. | 00 0.00 C |
| ATOM | 385 HA PROA | 30147.149 -12.925 | -5.631 1. | 00 0.00 H |
| ATOM | 386 1HB PRO A | 30148.902 -11.522 | -4.145 1.0 | 0.00 H |
| ATOM | 387 2HB PRO A | 30149.404 -12.446 | -5.567 1.0 | 00.00 H |
| ATOM | 388 1HG PROA | 30148.897 -9.508 | -5.296 1 | .00 0.00 Н |
| ATOM | 389 2HG PRO A | 30150.211 -10.344 | -6.145 1.0 | 00 0.00 H |
| ATOM | 390 1HD PRO A | 30148.006 -9.335 | -7.401 1 | .00 0.00 Н |
| ATOM | 391 2HD PRO A | 30148.927 -10.721 | -8.009 1. | 00 0.00 H |
| ATOM | 392 N PRO A | 31145.373 -11.959 | -4.095 1.0 | 00 0.00 N |
| ATOM | 393 CA PROA | 31144.428 -11.455 | -3.094 1. | 00 0.00 C |
| ATOM | 394 C PRO A | 31145.065 -11.310 | -1.717 1. | 00 0.00 C |
| ATOM | 395 O PRO A | 31144.943 -12.193 | -0.869 1. | 0 0.00 O |
| ATOM | 396 CB PROA | 31143.331 -12.523 | -3.065 1. | .00 0.00 C |
| ATOM | 397 CG PROA | 31143.999 -13.765 | -3.541 1. | .00 0.00 C |
| ATOM | 398 CD PROA | 31145.028 -13.322 | -4.543 1 | .00 0.00 C |
| ATOM | 399 HA PRO A | 31144.003 -10.507 | -3.393 1 | .00 0.00 Н |
| ATOM | 400 1HB PRO A | 31142.960 -12.634 | -2.057 1. | 00 0.00 H |
| ATOM | 401 2HB PRO A | 31142.524 -12.233 | -3.721 1. | 00 0.00 H |
| ATOM | 402 1HG PRO A | 31144.474 -14.268 | -2.712 1. | 00 0.00 H |

| ATOM | 403 2 | HG | PRO A | 31143.276 | -14.415 | -4.011 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 404 1 | | PRO A | 31145.892 | | -4.508 | 1.00 | 0.00 H |
| | 405 2 | | PRO A | 31143.607 | | -5.536 | 1.00 | 0.00 H |
| ATOM | | | | | | | | 0.00 N |
| ATOM | 406 | N | PHE A | 32145.746 | | -1.501 | 1.00 | |
| ATOM | 407 | CA | PHE A | 32146.404 | | -0.226 | 1.00 | 0.00 C |
| ATOM | 408 | С | PHE A | 32145.573 | -8.975 | 0.628 | 1.00 | 0.00 C |
| ATOM | 409 | О | PHE A | 32144.568 | -8.432 | 0.172 | 1.00 | 0.00 O |
| ATOM | 410 | CB | PHE A | 32147.798 | -9.342 | -0.457 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32147.825 | -8.245 | -1.484 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32147.160 | -7.051 | -1.259 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32148.516 | -8.409 | -2.674 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32147.184 | -6.040 | -2.201 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32148.543 | -7.402 | -3.620 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32147.875 | -6.216 | -3.383 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.807 | -9.522 | -2.217 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.501 | -10.868 | 0.295 | 1.00 | 0.00 H |
| ATOM | 419 1 | НВ | PHE A | 32148.168 | -8.935 | 0.471 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.460 | -10.127 | -0.791 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32146.618 | -6.912 | -0.335 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32149.038 | -9.336 | -2.860 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32146.660 | -5.114 | -2.014 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32149.085 | -7.543 | -4.543 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32147.895 | -5.428 | -4.122 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.003 | -8.777 | 1.870 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.297 | -7.889 | 2.789 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.273 | -6.965 | 3.508 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.259 | -7.417 | 4.092 | 1.00 | 0.00 O |
| | | | | | | | | |

| ATOM | 430 | CB | TYR A | 33144.502 | -8.706 | 3.809 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 431 | CG | TYR A | 33143.206 | -9.261 | 3.263 | 1.00 | 0.00 C |
| ATOM | .432 | CD1 | TYR A | 33142.351 | -8.466 | 2.509 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.838 - | 10.579 | 3.501 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.165 | -8.970 | 2.008 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.655 - | 11.090 | 3.002 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.822 | -10.282 | 2.257 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.643 | -10.787 | 1.759 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.811 | -9.238 | 2.178 | 1.00 | 0.00 H |
| ATOM | 439 | НА | TYR A | 33144.613 | -7.289 | 2.208 | 1.00 | 0.00 H |
| ATOM | 440 | НВ | TYR A | 33145.104 | -9.537 | 4.143 | 1.00 | 0.00 H |
| ATOM | 441 2 | 2HB | TYR A | 33144.264 | -8.077 | 4.655 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33142.623 | -7.439 | 2.316 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33143.492 | -11.209 | 4.086 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33140.515 | -8.336 | 1.424 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33141.386 - | -12.117 | 3.198 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.504 | -10.457 | 0.869 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.993 | -5.666 | 3.463 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.856 | -4.698 | 4.115 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34146.086 | -3.512 | 4.663 | 1.00 | 0.00 C |
| ATOM | 450 | O | GLY A | 34144.877 | - 3.403 | 4.464 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.194 | -5.363 | 2.983 | 1.00 | 0.00 H |
| ATOM | 452 | 1HA | GLY A | 34147.374 | -5.184 | 4.928 | 1.00 | 0.00 H |
| ATOM | 453 2 | 2HA | GLY A | 34147.583 | -4.342 | 3.400 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAĻ A | 35146.789 | -2.622 | 5.357 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VAL A | 35146.165 | -1.439 | 5.937 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.791 | -0.162 | 5.382 | 1.00 | 0.00 C |

| ATOM | 457 | O | VAL A | 35147.999 | -0.097 | 5.159 | 1.00 | 0.00 O |
|------|-----|------------|-------|-----------|--------|-------|------|--------|
| ATOM | 458 | СВ | VAL A | 35146.287 | -1.437 | 7.474 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VALA | 35147.746 | -1.405 | 7.899 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35145.523 | -0.263 | 8.071 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.751 | -2.766 | 5.482 | 1.00 | 0.00 H |
| ATOM | 462 | НА | VAL A | 35145.116 | -1.455 | 5.679 | 1.00 | 0.00 H |
| ATOM | 463 | НВ | VAL A | 35145.847 | -2.350 | 7.849 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VAL A | 35148.023 | -0.395 | 8.165 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35148.367 | -1.745 | 7.084 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VAL A | 35147.888 | -2.052 | 8.752 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VAL A | 35144.502 | -0.284 | 7.721 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VAL A | 35145.989 | 0.662 | 7.765 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VALA | 35145.537 | -0.335 | 9.148 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.958 | 0.852 | 5.164 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.430 | 2.126 | 4.637 | 1.00 | 0.00 C |
| ATOM | 472 | . C | ILE A | 36147.393 | 2.798 | 5.611 | 1.00 | 0.00 C |
| ATOM | 473 | O | ILE A | 36147.154 | 2.821 | 6.819 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.259 | 3.085 | 4.344 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.203 | 2.391 | 3.480 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILE A | 36145.765 | 4.346 | 3.658 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36143.021 | 3.272 | 3.144 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36145.006 | 0.739 | 5.363 | 1.00 | 0.00 H |
| ATOM | 479 | НА | ILE A | 36146.950 | 1.932 | 3.710 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.813 | 3.371 | 5.284 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.657 | 2.077 | 2.552 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.832 | 1.522 | 4.005 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36144.985 | 5.093 | 3.655 | 1.00 | 0.00 H |

| ATOM | 484 2HG2 | ILEA 3 | 36146.045 | 4.115 | 2.640 | 1.00 |).00 H |
|------|----------|---------|-----------|-------|--------|------|--------|
| ATOM | 485 3HG2 | ILE A 3 | 36146.625 | 4.726 | 4.190 | 1.00 |).00 H |
| ATOM | 486 1HD1 | ILE A 3 | 36143.302 | 4.309 | 3.253 | 1.00 |).00 H |
| ATOM | 487 2HD1 | ILE A 3 | 36142.203 | 3.047 | 3.812 | 1.00 | H 00.0 |
| ATOM | 488 3HD1 | ILE A | 36142.713 | 3.089 | 2.125 | 1.00 | H 00.0 |
| ATOM | 489 N | ARG A | 37148.482 | 3.342 | 5.078 | 1.00 | 0.00 N |
| ATOM | 490 CA | ARG A | 37149.482 | 4.013 | 5.901 | 1.00 | 0.00 C |
| ATOM | 491 C | ARG A | 37149.654 | 5.467 | 5.474 | 1.00 | 0.00 C |
| ATOM | 492 O | ARG A | 37149.380 | 6.387 | 6.245 | 1.00 | 0.00 O |
| ATOM | 493 CB | ARG A | 37150.821 | 3.279 | 5.811 | 1.00 | 0.00 C |
| ATOM | 494 CG | ARG A | 37150.720 | 1.790 | 6.099 | 1.00 | 0.00 C |
| ATOM | 495 CD | ARG A | 37150.093 | 1.526 | 7.458 | 1.00 | 0.00 C |
| ATOM | 496 NE | ARG A | 37150.689 | 2.353 | 8.506 | 1.00 | 0.00 N |
| ATOM | 497 CZ | ARG A | 37150.129 | 2.558 | 9.696 | 1.00 | 0.00 C |
| ATOM | 498 NH1 | ARG A | 37148.963 | 1.999 | 9.993 | 1.00 | 0.00 N |
| ATOM | 499 NH2 | 2 ARG A | 37150.737 | 3.323 | 10.591 | 1.00 | 0.00 N |
| ATOM | 500 H | ARG A | 37148.617 | 3.291 | 4.109 | 1.00 | 0.00 H |
| ATOM | 501 HA | ARG A | 37149.138 | 3.991 | 6.924 | 1.00 | 0.00 H |
| ATOM | 502 1HB | ARG A | 37151.221 | 3.405 | 4.816 | 1.00 | 0.00 H |
| ATOM | 503 2HB | ARG A | 37151.507 | 3.716 | 6.522 | 1.00 | 0.00 H |
| ATOM | 504 1HG | ARG A | 37150.112 | 1.327 | 5.337 | 1.00 | 0.00 H |
| ATOM | 505 2HG | ARG A | 37151.712 | 1.362 | 6.079 | 1.00 | 0.00 H |
| ATOM | 506 1HD | ARG A | 37149.036 | 1.741 | 7.401 | 1.00 | 0.00 H |
| ATOM | 507 2HD | ARG A | 37150.235 | 0.486 | 7.710 | 1.00 | 0.00 H |
| ATOM | 508 HE | ARG A | 37151.550 | 2.778 | 8.311 | 1.00 | 0.00 H |
| ATOM | 509 1HH1 | ARG A | 37148.498 | 1.422 | 9.322 | 1.00 | 0.00 H |
| ATOM | 510 2HH1 | ARG A | 37148.547 | 2.158 | 10.889 | 1.00 | 0.00 H |

| ATOM | 511 1 | нна. | ARG A | 37151.617 | 3.746 | 10.372 | 1.00 | 0.00 H |
|--------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | | | ARG A | 37150.318 | 3.477 | 11.485 | 1.00 | 0.00 H |
| ATOM | 512 2 | N | TRPA | 38150.112 | 5.667 | 4.242 | 1.00 | 0.00 N |
| | | | | | 7.011 | 3.714 | 1.00 | 0.00 C |
| ATOM | 514 | CA | TRPA | 38150.321 | | | | |
| ATOM | 515 | C | TRPA | 38149.551 | 7.213 | 2.412 | 1.00 | 0.00 C |
| ATOM | 516 | 0 | TRPA | 38149.601 | 6.374 | 1.511 | 1.00 | 0.00 O |
| ATOM | 517 | CB | TRPA | 38151.814 | 7.269 | 3.486 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38152.095 | 8.525 | 2.714 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRPA | 38152.313 | 9.772 | 3.226 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRP A | 38152.181 | 8.655 | 1.290 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRP A | 38152.531 | 10.669 | 2.207 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.455 | 10.006 | 1.009 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38152.055 | 7.758 | 0.225 | 1.00 | 0.00 C |
| ATOM - | 524 | CZ2 | TRPA | 38152.603 | 10.481 | -0.292 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRP A | 38152.202 | 8.230 | -1.066 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRP A | 38152.474 | 9.581 | -1.315 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRPA | 38150.313 | 4.895 | 3.674 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRP A | 38149.952 | 7.715 | 4.446 | 1.00 | 0.00 H |
| ATOM | 529 1 | НВ | TRPA | 38152.309 | 7.350 | 4.443 | 1.00 | 0.00 H |
| ATOM | 530 2 | HB | TRPA | 38152.236 | 6.439 | 2.938 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38152.312 | 10.006 | 4.280 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38152.711 | 11.625 | 2.319 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRPA | 38151.845 | 6.713 | 0.397 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38152.809 | 11.521 | -0.501 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.108 | 7.552 | -1.900 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRPA | 38152.582 | 9.906 | -2.340 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.850 | 8.337 | 2.318 | 1.00 | 0.00 N |

| ATOM | 538 | CA | ILE A | 39148.078 | 8.664 | 1.126 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 539 | C | ILE A | 39148.492 | 10.024 | 0.575 | 1.00 | 0.00 C |
| ATOM | 540 | О | ILE A | 39148.159 | 11.062 | 1.146 | 1.00 | 0.00 O |
| ATOM | 541 | СВ | ILE A | 39146.566 | 8.679 | 1.420 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39146.151 | 7.396 | 2.143 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILEA | 39145.777 | 8.844 | 0.129 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.691 | 7.371 | 2.539 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.859 | 8.968 | 3.067 | 1.00 | 0.00 H |
| ATOM | 546 | НА | ILE A | 39148.275 | 7.907 | 0.380 | 1.00 | 0.00 H |
| ATOM | 547 | НВ | ILE A | 39146.353 | 9.526 | 2.053 | 1.00 | 0.00 H |
| ATOM | 548 | 1HG1 | ILE A | 39146.334 | 6.551 | 1.496 | 1.00 | 0.00 H |
| ATOM | 549 | 2HG1 | ILE A | 39146.742 | 7.290 | 3.041 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39144.765 | 8.499 | 0.279 | 1.00 | 0.00 H |
| ATOM | 551 | 2HG2 | ILE A | 39146.242 | 8.264 | -0.654 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39145.764 | 9.886 | -0.154 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.182 | 8.211 | 2.090 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39144.608 | 7.431 | 3.614 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39144.241 | 6.451 | 2.194 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.226 | 10.012 | -0.532 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.678 | 11.253 | -1.131 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.185 | 11.072 | -2.546 | 1.00 | 0.00 C |
| ATOM | 559 | Ο | GLY A | 40150.020 | 10.007 | -3.142 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.467 | 9.155 | -0.943 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40148.858 | 11.955 | -1.141 | 1.00 | 0.00 H |
| ATOM | 562 | 2HA | GLY A | 40150.474 | 11.659 | -0.526 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41150.799 | 12.118 | -3.087 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.332 | 12.082 | -4.441 | 1.00 | 0.00 C |

| 4TO 1 6 | | _ | CLNIA | 41150 704 | 12.520 | 4.460 | 1.00 | 0.00 C |
|---------|-------|------|-------|-----------|--------|---------|------|--------|
| ATOM | 565 | С | GLN A | | 12.528 | -4.460 | 1.00 | |
| ATOM | 566 | О | GLN A | 41153.100 | 13.680 | -4.154 | 1.00 | 0.00 O |
| ATOM | 567 | CB | GLN A | 41150.498 | 12.981 | -5.353 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41149.001 | 12.756 | -5.223 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.213 | 14.050 | -5.269 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.200 | 14.818 | -4.307 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41147.549 | 14.296 | -6.391 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41150.896 | 12.939 | -2.561 | 1.00 | 0.00 H |
| ATOM | 573 | НА | GLN A | 41151.268 | 11.065 | -4.798 | 1.00 | 0.00 H |
| ATOM | 574 | 1HB | GLN A | 41150.707 | 14.011 | - 5.111 | 1.00 | 0.00 H |
| ATOM | 575 2 | 2HB | GLN A | 41150.782 | 12.797 | -6.377 | 1.00 | 0.00 H |
| ATOM | 576 | 1HG | GLN A | 41148.673 | 12.124 | -6.034 | 1.00 | 0.00 H |
| ATOM | 577 | 2HG | GLN A | 41148.803 | 12.265 | -4.282 | 1.00 | 0.00 H |
| ATOM | 578 | 1HE2 | GLN A | 41147.606 | 13.638 | -7.115 | 1.00 | 0.00 H |
| ATOM | 579 | 2HE2 | GLN A | 41147.032 | 15.126 | -6.451 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42153.720 | 11.620 | -4.817 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.153 | 11.933 | -4.868 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.457 | 13.100 | -5.803 | 1.00 | 0.00 C |
| ATOM | 583 | O | PRO A | 42154.658 | 13.428 | -6.681 | 1.00 | 0.00 O |
| ATOM | 584 | СВ | PRO A | 42155.789 | 10.645 | -5.399 | 1.00 | 0.00 C |
| ATOM | 585 | CG | PRO A | 42154.802 | 9.575 | -5.083 | 1.00 | 0.00 C |
| ATOM | 586 | CD | PRO A | 42153.453 | 10.221 | -5.197 | 1.00 | 0.00 C |
| ATOM | 587 | НА | PRO A | 42155.544 | 12.152 | -3.885 | 1.00 | 0.00 H |
| ATOM | 588 | 1HB | PRO A | 42155.950 | 10.733 | -6.465 | 1.00 | 0.00 H |
| ATOM | 589 | 2HB | PRO A | 42156.731 | 10.472 | -4.900 | 1.00 | 0.00 H |
| ATOM | 590 | 1HG | PRO A | 42154.894 | 8.767 | -5.794 | 1.00 | 0.00 H |
| ATOM | 591 | 2HG | PRO A | 42154.961 | 9.213 | -4.078 | 1.00 | 0.00 H |
| | | | | | | | | |

| ATOM | 592 1HD | PRO A | 42153.088 | 10.159 | -6.213 | 1.00 | 0.00 H |
|------|---------|-------|-----------|----------|---------|------|--------|
| ATOM | 593 2HD | PRO A | 42152.754 | 9.763 | -4.513 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43156.621 | 13.746 | -5.625 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.028 | 14.881 | -6.457 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43157.418 | 14.454 | -7.866 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43158.590 | 14.200 | -8.146 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43158.241 | 15.445 | -5.719 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43158.803 | 14.285 | -4.973 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43157.630 | 13.420 | -4.600 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43156.254 | 15.632 | -6.510 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43158.948 | 15.836 | -6.435 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43157.926 | 16.230 | -5.048 | 1.00 | 0.00 H |
| ATOM | 604 1HG | PRO A | 43159.487 | 13.738 | -5.607 | 1.00 | 0.00 H |
| ATOM | 605 2HG | PRO A | 43159.311 | 14.631 | -4.085 | 1.00 | 0.00 H |
| ATOM | 606 1HD | PRO A | 43157.903 | 12.376 | -4.647 | 1.00 | 0.00 H |
| ATOM | 607 2HD | PRO A | 43157.273 | 13.673 | -3.614 | 1.00 | 0.00 H |
| ATOM | 608 N | GLY A | 44156.432 | 14.379 | -8.752 | 1.00 | 0.00 N |
| ATOM | 609 CA | GLY A | 44156.696 | 13.984 | -10.122 | 1.00 | 0.00 C |
| ATOM | 610 C | GLY A | 44155.463 | 13.450 - | 10.820 | 1.00 | 0.00 C |
| ATOM | 611 O | GLY A | 44155.131 | 13.883 - | 11.924 | 1.00 | 0.00 O |
| ATOM | 612 H | GLY A | 44155.517 | 14.595 | -8.473 | 1.00 | 0.00 H |
| ATOM | 613 1HA | GLY A | 44157.062 | 14.839 - | 10.667 | 1.00 | 0.00 H |
| ATOM | 614 2HA | GLY A | 44157.457 | 13.216 - | 10.121 | 1.00 | 0.00 H |
| ATOM | 615 N | LEU A | 45154.782 | 12.507 | -10.178 | 1.00 | 0.00 N |
| ATOM | 616 CA | LEU A | 45153.577 | 11.916 | -10.749 | 1.00 | 0.00 C |
| ATOM | 617 C | LEU A | 45152.383 | 12.121 | -9.826 | 1.00 | 0.00 C |
| ATOM | 618 O | LEU A | 45152.330 | 11.557 | -8.733 | 1.00 | 0.00 O |

| | - 127 | - |
|------|--------------------------|----------------------------|
| ATOM | (10 CD LEUA 45152.790 | 10.422 -11.006 1.00 0.00 C |
| ATOM | 619 CB LEUA 45153.789 | |
| ATOM | | 9.647 -9.841 1.00 0.00 C |
| ATOM | 621 CD1 LEU A 45154.115 | 8.159 -9.974 1.00 0.00 C |
| ATOM | 622 CD2 LEU A 45155.907 | 9.898 -9.771 1.00 0.00 C |
| ATOM | 623 H LEUA 45155.095 | 12.205 -9.298 1.00 0.00 H |
| ATOM | 624 HA LEUA 45153.380 | 12.409 -11.690 1.00 0.00 H |
| ATOM | 625 1HB LEU A 45152.830 | 9.980 -11.238 1.00 0.00 H |
| ATOM | 626 2HB LEU A 45154.434 | 10.314 -11.865 1.00 0.00 H |
| ATOM | 627 HG LEUA 45153.966 | 9.991 -8.916 1.00 0.00 H |
| ATOM | 628 1HD1 LEU A 45155.036 | 7.624 -10.154 1.00 0.00 H |
| ATOM | 629 2HD1 LEU A 45153.438 | 7.995 -10.800 1.00 0.00 H |
| ATOM | 630 3HD1 LEU A 45153.663 | 7.798 -9.062 1.00 0.00 H |
| ATOM | 631 1HD2 LEU A 45156.426 | 8.959 -9.648 1.00 0.00 H |
| ATOM | 632 2HD2 LEU A 45156.125 | 10.542 -8.932 1.00 0.00 H |
| ATOM | 633 3HD2 LEU A 45156.236 | 10.374 -10.684 1.00 0.00 H |
| ATOM | 634 N ASNA 46151.424 | 12.927 -10.269 1.00 0.00 N |
| ATOM | 635 CA ASN A 46150.235 | 13.193 -9.470 1.00 0.00 C |
| ATOM | 636 C ASN A 46149.317 | 11.976 -9.459 1.00 0.00 C |
| ATOM | 637 O ASN A 46148.674 | 11.660 -10.460 1.00 0.00 O |
| ATOM | 638 CB ASNA 46149.488 | 14.408 -10.023 1.00 0.00 C |
| ATOM | 639 CG ASN A 46148.414 | 14.909 -9.078 1.00 0.00 C |
| ATOM | 640 OD1 ASN A 46147.337 | 14.320 -8.976 1.00 0.00 O |
| ATOM | 641 ND2 ASN A 46148.701 | 16.002 -8.381 1.00 0.00 N |
| ATOM | 642 H ASNA 46151.517 | 13.350 -11.148 1.00 0.00 H |
| ATOM | 643 HA ASN A 46150.552 | |
| ATOM | 644 1HB ASN A 46150.192 | 15.210 -10.193 1.00 0.00 H |
| | | 14.140 -10.960 1.00 0.00 H |
| ATOM | 645 2HB ASN A 46149.022 | 17.170 -10.700 1.00 0.0011 |

| ATOM | 646 | HD2 | ASN A | 46149.578 | 16.418 | -8.513 | 1.00 | 0.00 H | |
|------|-------|------|-------|-----------|---------|---------|------|--------|--|
| ATOM | 647 2 | 2HD2 | ASN A | 46148.024 | 16.347 | -7.762 | 1.00 | 0.00 H | |
| ATOM | 648 | N | GLU A | 47149.262 | 11.298 | -8.318 | 1.00 | 0.00 N | |
| ATOM | 649 | CA | GLU A | 47148.424 | 10.115 | -8.169 | 1.00 | 0.00 C | |
| ATOM | 650 | C | GLU A | 47148.293 | 9.726 | -6.701 | 1.00 | 0.00 C | |
| ATOM | 651 | О | GLU A | 47149.290 | 9.450 | -6.033 | 1.00 | 0.00 O | |
| ATOM | 652 | CB | GLU A | 47149.005 | 8.945 | -8.967 | 1.00 | 0.00 C | |
| ATOM | 653 | CG | GLU A | 47150.523 | 8.861 | -8.914 | 1.00 | 0.00 C | |
| ATOM | 654 | CD | GLU A | 47151.092 | 7.924 | -9.962 | 1.00 | 0.00 C | |
| ATOM | 655 | OE1 | GLU A | 47151.464 | 6.787 | -9.603 | 1.00 | 0.00 O | |
| ATOM | 656 | OE2 | GLU A | 47151.164 | 8.328 - | 11.142 | 1.00 | 0.00 O | |
| ATOM | 657 | Н | GLU A | 47149.799 | 11.601 | -7.558 | 1.00 | 0.00 H | |
| ATOM | 658 | HA | GLU A | 47147.445 | 10.351 | -8.555 | 1.00 | 0.00 H | |
| ATOM | 659 | 1HB | GLU A | 47148.602 | 8.022 | -8.577 | 1.00 | 0.00 H | |
| ATOM | 660 2 | 2HB | GLU A | 47148.709 | 9.048 | -10.001 | 1.00 | 0.00 H | |
| ATOM | 661 | 1HG | GLU A | 47150.931 | 9.847 | -9.076 | 1.00 | 0.00 H | |
| ATOM | 662 | 2HG | GLU A | 47150.820 | 8.507 | -7.938 | 1.00 | 0.00 H | |
| ATOM | 663 | N | VAL A | 48147.064 | 9.696 | -6.203 | 1.00 | 0.00 N | |
| ATOM | 664 | CA | VAL A | 48146.817 | 9.330 | -4.815 | 1.00 | 0.00 C | |
| ATOM | 665 | C | VALA | 48147.192 | 7.874 | -4.570 | 1.00 | 0.00 C | |
| ATOM | 666 | О | VAL A | 48146.430 | 6.963 | -4.895 | 1.00 | 0.00 O | |
| ATOM | 667 | СВ | VAL A | 48145.342 | 9.544 | -4.426 | 1.00 | 0.00 C | |
| ATOM | 668 | CG1 | VAL A | 48145.152 | 9.357 | -2.928 | 1.00 | 0.00 C | |
| ATOM | 669 | CG2 | VALA | 48144.869 | 10.922 | -4.863 | 1.00 | 0.00 C | |
| ATOM | 670 | Н | VAL A | 48146.305 | 9.918 | -6.782 | 1.00 | 0.00 H | |
| ATOM | 671 | HA | VAL A | 48147.433 | 9.961 | -4.188 | 1.00 | 0.00 H | |
| ATOM | 672 | НВ | VAL A | 48144.745 | 8.803 | -4.936 | 1.00 | 0.00 H | |

| ATOM | 673 1HG1 | VALA | 48144.216 | 9.803 | -2.627 | 1.00 | 0.00 H |
|------|----------|-------|-----------|--------|--------|------|--------|
| ATOM | 674 2HG1 | VALA | 48145.964 | 9.833 | -2.401 | 1.00 | 0.00 H |
| ATOM | 675 3HG1 | VAL A | 48145.140 | 8.302 | -2.696 | 1.00 | 0.00 H |
| ATOM | 676 1HG2 | VALA | 48145.632 | 11.653 | -4.636 | 1.00 | 0.00 H |
| ATOM | 677 2HG2 | VALA | 48143.961 | 11.174 | -4.337 | 1.00 | 0.00 H |
| ATOM | 678 3HG2 | VALA | 48144.681 | 10.918 | -5.926 | 1.00 | 0.00 H |
| ATOM | 679 N | LEU A | 49148.373 | 7.660 | -4.000 | 1.00 | 0.00 N |
| ATOM | 680 CA | LEU A | 49148.852 | 6.313 | -3.717 | 1.00 | 0.00 C |
| ATOM | 681 C | LEU A | 49148.792 | 6.021 | -2.223 | 1.00 | 0.00 C |
| ATOM | 682 O | LEU A | 49149.500 | 6.641 | -1.431 | 1.00 | 0.00 O |
| ATOM | 683 · CB | LEU A | 49150.283 | 6.140 | -4.227 | 1.00 | 0.00 C |
| ATOM | 684 CG | LEU A | 49150.454 | 6.288 | -5.740 | 1.00 | 0.00 C |
| ATOM | 685 CD1 | LEU A | 49151.838 | 6.822 | -6.071 | 1.00 | 0.00 C |
| ATOM | 686 CD2 | LEU A | 49150.214 | 4.956 | -6.434 | 1.00 | 0.00 C |
| ATOM | 687 H | LEU A | 49148.937 | 8.425 | -3.765 | 1.00 | 0.00 H |
| ATOM | 688 HA | LEU A | 49148.208 | 5.617 | -4.234 | 1.00 | 0.00 H |
| ATOM | 689 1HB | LEU A | 49150.907 | 6.878 | -3.741 | 1.00 | 0.00 H |
| ATOM | 690 2HB | LEU A | 49150.629 | 5.158 | -3.942 | 1.00 | 0.00 H |
| ATOM | 691 HG | LEU A | 49149.726 | 6.995 | -6.111 | 1.00 | 0.00 H |
| ATOM | 692 1HD1 | LEU A | 49151.800 | 7.900 | -6.146 | 1.00 | 0.00 H |
| ATOM | 693 2HD1 | LEU A | 49152.169 | 6.408 | -7.012 | 1.00 | 0.00 H |
| ATOM | 694 3HD1 | LEU A | 49152.530 | 6.540 | -5.290 | 1.00 | 0.00 H |
| ATOM | 695 1HD2 | LEU A | 49149.181 | 4.891 | -6.742 | 1.00 | 0.00 H |
| ATOM | 696 2HD2 | LEU A | 49150.438 | 4.149 | -5.751 | 1.00 | 0.00 H |
| ATOM | 697 3HD2 | LEU A | 49150.854 | 4.882 | -7.301 | 1.00 | 0.00 H |
| ATOM | 698 N | ALAA | 50147.943 | 5.072 | -1.846 | 1.00 | 0.00 N |
| ATOM | 699 CA | ALA A | 50147.794 | 4.702 | -0.446 | 1.00 | 0.00 C |

| ATOM | 700 | C | ALA A | 50148.728 | 3.553 | -0.081 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|---------|------|--------|
| ATOM | 701 | О | ALA A | 50148.587 | 2.440 | -0.588 | 1.00 | 0.00 O |
| ATOM | 702 | СВ | ALA A | 50146.350 | 4.325 | - 0.152 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.405 | 4.613 | -2.524 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50148.047 | 5.565 | 0.151 | 1.00 | 0.00 H |
| ATOM | 705 1 | НВ | ALA A | 50145.908 | 3.878 | -1.029 | 1.00 | 0.00 H |
| ATOM | 706 2 | 2HB | ALA A | 50145.795 | 5.211 | 0.119 | 1.00 | 0.00 H |
| ATOM | 707 3 | ВНВ | ALA A | 50146.321 | 3.620 | 0.666 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.682 | 3.830 | 0.801 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.625 | 2.809 | 1.219 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51149.976 | 1.735 | 2.070 | 1.00 | 0.00 C |
| ATOM | 711 | О | GLY A | 51149.657 | 1.965 | 3.236 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.746 | 4.734 | 1.173 | 1.00 | 0.00 H |
| ATOM | 713 | lΗA | GLY A | 51151.052 | 2.348 | 0.341 | 1.00 | 0.00 H |
| ATOM | 714 2 | 2HA | GLY A | 51151.414 | 3.275 | 1.789 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.779 | 0.557 | 1.485 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.164 | -0.556 | 2.198 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.224 | -1.465 | 2.808 | 1.00 | 0.00 C |
| ATOM | 718 | O | LEU A | 52151.150 | -1.902 | 2.125 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.265 | -1.358 | 1.256 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.001 | -0.634 | 0.792 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.360 | -1.372 | -0.373 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52146.016 | -0.493 | 1.943 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.054 | 0.434 | 0.553 | 1.00 | 0.00 H |
| ATOM | 724 | НА | LEU A | 52148.559 | -0.145 | 2.994 | 1.00 | 0.00 H |
| ATOM | 725 | lНВ | LEU A | 52148.844 | -1.626 | 0.383 | 1.00 | 0.00 H |
| ATOM | 726 2 | 2HB | LEU A | 52147.968 | -2.266 | 1.761 | 1.00 | 0.00 H |

| ATOM | 727 | HG | LEU A | 52147.265 | 0.358 | 0.453 | 1.00 | 0.00 H |
|------|-----|------|---------|-----------|--------|--------|------|--------|
| ATOM | 728 | 1HD1 | LEU A | 52146.068 | -2.362 | -0.055 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52147.069 | -1.448 | -1.184 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52145.488 | -0.829 | -0.707 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52145.198 | 0.145 | 1.641 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52146.517 | -0.057 | 2.794 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52145.633 | -1.467 | 2.211 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53150.082 | -1.748 | 4.100 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53151.027 | -2.607 | 4.802 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.520 | -4.044 | 4.856 | 1.00 | 0.00 C |
| ATOM | 737 | Ο | GLU A | 53149.535 | -4.340 | 5.532 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.266 | -2.085 | 6.221 | 1.00 | 0.00 C |
| ATOM | 739 | CG | GLU A | 53152.268 | -2.908 | 7.013 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.835 | -3.131 | 8.448 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53151.291 | -4.216 | 8.744 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | 2 GLU A | 53152.041 | -2.220 | 9.279 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53149.323 | -1.370 | 4.591 | 1.00 | 0.00 H |
| ATOM | 744 | HA | GLU A | 53151.961 | -2.587 | 4.259 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.633 | -1.071 | 6.162 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53150.327 | -2.087 | 6.756 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53152.382 | -3.870 | 6.534 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53153.217 | -2.393 | 7.013 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54151.200 | -4.933 | 4.139 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.817 | -6.340 | 4.105 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54151.111 | -7.016 | 5.440 | 1.00 | 0.00 C |
| ATOM | 752 | 0 | LEU A | 54152.156 | -6.782 | 6.049 | 1.00 | 0.00 O |
| ATOM | 753 | СВ | LEU A | 54151.558 | -7.064 | 2.979 | 1.00 | 0.00 C |

| ATOM | 754 | CG | LEU A | 54151.517 | -6.362 | 1.621 | 1.00 | 0.00 C |
|-------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 755 | CD1 | LEU A | 54152.750 | -6.710 | 0.802 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54150.250 | -6.737 | 0.867 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.976 | -4.637 | 3.621 | 1.00 | 0.00 H |
| ATOM: | 758 | HA | LEU A | 54149.755 | -6.390 | 3.916 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.592 | -7.178 | 3.272 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54151.123 | -8.046 | 2.864 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.510 | -5.293 | 1.776 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54152.593 | -6.419 | -0.226 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54152.926 | -7.775 | 0.853 | 1.00 | 0.00 H |
| ATOM | 764 | 3HD1 | LEU A | 54153.605 | -6.184 | 1.199 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54150.238 | -7.803 | 0.691 | 1.00 | 0.00 H |
| ATOM | 766 | 2HD2 | LEU A | 54150.227 | -6.216 | -0.080 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.386 | -6.459 | 1.452 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55150.185 | -7.857 | 5.890 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55150.346 | -8.568 | 7.153 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55151.400 | -9.662 | 7.031 | 1.00 | 0.00 C |
| ATOM | 771 | O | GLU A | 55152.098 | -9.977 | 7.995 | 1.00 | 0.00 O |
| ATOM | 772 | СВ | GLU A | 55149.013 | -9.174 | 7.594 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55148.076 | -8.172 | 8.249 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55146.632 | -8.363 | 7.827 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55145.767 | -8.503 | 8.717 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55146.366 | -8.371 | 6.606 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.374 | -8.002 | 5.359 | 1.00 | 0.00 H |
| ATOM | 778 | HA | GLU A | 55150.670 | -7.853 | 7.895 | 1.00 | 0.00 H |
| ATOM | 779 | 1HB | GLU A | 55148.515 | -9.588 | 6.730 | 1.00 | 0.00 H |
| ATOM | 780 | 2HB | GLU A | 55149.207 | -9.967 | 8.301 | 1.00 | 0.00 H |

| ATOM | 781 | HG | GLU A | 55148.139 | -8.286 | 9.321 | 1.00 | 0.00 H |
|------|-------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 782 2 | 2HG | GLU A | 55148.387 | -7.174 | 7.974 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASP A | 56151.511 - | 10.239 | 5.839 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASPA | 56152.481 - | -11.300 | 5.590 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASP A | 56153.770 - | 10.732 | 5.004 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASP A | 56153.744 - | 10.008 | 4.008 | 1.00 | 0.00 O |
| ATOM | 787 | СВ | ASPA | 56151.893 - | 12.345 | 4.642 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56151.185 | -13.464 | 5.381 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASP A | 56151.383 - | 14.640 | 5.009 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASP A | 56150.434 - | 13.164 | 6.333 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASP A | 56150.927 | -9.945 | 5.109 | 1.00 | 0.00 H |
| ATOM | 792 | HA | ASPA | 56152.707 | -11.770 | 6.535 | 1.00 | 0.00 H |
| ATOM | 793 1 | НВ | ASPA | 56151.181 - | 11.867 | 3.985 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASPA | 56152.688 - | 12.775 | 4.051 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.895 | -11.065 | 5.626 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57156.194 | -10.588 | 5.166 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.577 | -11.245 | 3.845 | 1.00 | 0.00 C |
| ATOM | 798 | Ο . | GLU A | 57157.029 | -12.390 | 3.817 | 1.00 | 0.00 O |
| ATOM | 799 | CB | GLU A | 57157.267 | -10.870 | 6.220 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.447 | -9.740 | 7.221 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57158.872 | -9.634 | 7.728 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57159.805 | -9.697 | 6.900 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57159.056 | -9.488 | 8.955 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.851 | -11.645 | 6.416 | 1.00 | 0.00 H |
| ATOM | 805 | НА | GLU A | 57156.121 | -9.522 | 5.016 | 1.00 | 0.00 H |
| ATOM | 806 | НВ | GLU A | 57156.996 | -11.764 | 6.763 | 1.00 | 0.00 H |
| ATOM | 807 2 | 2HB | GLU A | 57158.211 | -11.035 | 5.721 | 1.00 | 0.00 H |

| ATOM | 808 1HG | GLU A | 57157.181 -8.809 | 6.746 | 1.00 | 0.00 H |
|------|---------|--------|-------------------|--------|------|--------|
| ATOM | 809 2HG | GLU A | 57156.793 -9.914 | 8.062 | 1.00 | 0.00 H |
| ATOM | 810 N | CYS A. | 58156.395 -10.513 | 2.750 | 1.00 | 0.00 N |
| ATOM | 811 CA | CYS A | 58156.722 -11.025 | 1.425 | 1.00 | 0.00 C |
| ATOM | 812 C | CYS A | 58158.004 -10.389 | 0.898 | 1.00 | 0.00 C |
| ATOM | 813 O | CYS A | 58158.094 -9.169 | 0.762 | 1.00 | 0.00 O |
| ATOM | 814 CB | CYS A | 58155.570 -10.760 | 0.454 | 1.00 | 0.00 C |
| ATOM | 815 SG | CYS A | 58154.347 -12.089 | 0.379 | 1.00 | 0.00 S |
| ATOM | 816 H | CYSA | 58156.032 -9.607 | 2.837 | 1.00 | 0.00 H |
| ATOM | 817 HA | CYS A | 58156.872 -12.091 | 1.509 | 1.00 | 0.00 H |
| ATOM | 818 1HB | CYS A | 58155.057 -9.858 | 0.754 | 1.00 | 0.00 H |
| ATOM | 819 2HB | CYS A | 58155.972 -10.625 | -0.540 | 1.00 | 0.00 H |
| ATOM | 820 HG | CYS A | 58154.819 -12.920 | 0.284 | 1.00 | 0.00 H |
| ATOM | 821 N | ALA A | 59158.995 -11.225 | 0.602 | 1.00 | 0.00 N |
| ATOM | 822 CA | ALA A | 59160.272 -10.744 | 0.090 | 1.00 | 0.00 C |
| ATOM | 823 C | ALA A | 59160.092 -10.017 | -1.238 | 1.00 | 0.00 C |
| ATOM | 824 O | ALA A | 59159.556 -10.575 | -2.195 | 1.00 | 0.00 O |
| ATOM | 825 CB | ALA A | 59161.246 -11.902 | -0.069 | 1.00 | 0.00 C |
| ATOM | 826 H | ALA A | 59158.864 -12.187 | 0.732 | 1.00 | 0.00 H |
| ATOM | 827 HA | ALA A | 59160.683 -10.055 | 0.813 | 1.00 | 0.00 H |
| ATOM | 828 1HB | ALA A | 59161.919 -11.697 | -0.889 | 1.00 | 0.00 H |
| ATOM | 829 2HB | ALA A | 59160.697 -12.809 | -0.272 | 1.00 | 0.00 H |
| ATOM | 830 3HB | ALA A | 59161.814 -12.021 | 0.841 | 1.00 | 0.00 H |
| ATOM | 831 N | GLY A | 60160.541 -8.767 | -1.288 | 1.00 | 0.00 N |
| ATOM | 832 CA | GLY A | 60160.420 -7.984 | -2.504 | 1.00 | 0.00 C |
| ATOM | 833 C | GLY A | 60159.945 -6.569 | -2.237 | 1.00 | 0.00 C |
| ATOM | 834 O | GLY A | 60160.265 - 5.647 | -2.989 | 1.00 | 0.00 O |

| ATOM | 835 | Н | GLY A | 60160.959 | -8.373 | -0.494 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 836 | 1HA | GLY A | 60161.382 | -7.943 | -2.991 | 1.00 | 0.00 H |
| ATOM | 837 | 2HA | GLY A | 60159.715 | -8.469 | -3.163 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61159.183 | -6.395 | -1.163 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.664 | -5.082 | -0.798 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.626 | -4.359 | 0.140 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.633 | -4.922 | 0.567 | 1.00 | 0.00 O |
| ATOM | 842 | CB | CYS A | 61157.293 | -5.218 | -0.136 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYSA | 61156.080 | -6.119 | -1.129 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.963 | -7.168 | -0.602 | 1.00 | 0.00 H |
| ATOM | 845 | HA | CYS A | 61158.561 | -4.503 | -1.704 | 1.00 | 0.00 H |
| ATOM | 846 | 1HB | CYS A | 61157.403 | -5.742 | 0.801 | 1.00 | 0.00 H |
| ATOM | 847 | 2HB | CYS A | 61156.894 | -4.232 | 0.055 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61156.127 | -5.787 | -2.029 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62159.306 | -3.107 | 0.457 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62160.142 | -2.308 | 1.345 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.530 | -2.225 | 2.739 | 1.00 | 0.00 C |
| ATOM | 852 | Ο | THR A | 62158.568 | -2.929 | 3.048 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62160.329 | -0.902 | 0.774 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62159.146 | -0.138 | 0.925 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.696 | -0.896 | -0.695 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62158.490 | -2.714 | 0.084 | 1.00 | 0.00 H |
| ATOM | 857 | HA | THR A | 62161.106 | -2.789 | 1.416 | 1.00 | 0.00 H |
| ATOM | 858 | HB | THR A | 62161.123 | -0.407 | 1.314 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62158.400 | -0.629 | 0.572 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62161.182 | 0.036 | -0.941 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62159.800 | -1.003 | -1.290 | 1.00 | 0.00 H |

| ATOM | 862 | 3HG2 | THR A | 62161.365 | -1.718 | -0.902 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 863 | N | ASPA | 63160.095 | -1.362 | 3.578 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASPA | 63159.605 | -1.188 | 4.940 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASP A | 63158.822 | 0.115 | 5.073 | 1.00 | 0.00 C |
| ATOM | 866 | Ο | ASP A | 63158.815 | 0.740 | 6.134 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASPA | 63160.772 | -1.199 | 5.930 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.778 | -0.100 | 5.649 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63162.909 | -0.422 | 5.230 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63161.434 | 1.085 | 5.850 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASPA | 63160.860 | -0.830 | 3.272 | 1.00 | 0.00 H |
| ATOM | 872 | HA | ASPA | 63158.947 | -2.013 | 5.164 | 1.00 | 0.00 H |
| ATOM | 873 | 1HB | ASPA | 63160.389 | -1.064 | 6.930 | 1.00 | 0.00 H |
| ATOM | 874 | 2HB | ASPA | 63161.279 | -2.151 | 5.867 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64158.166 | 0.519 | 3.991 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.389 | 1.744 | 4.009 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64158.114 | 2.900 | 3.347 | 1.00 | 0.00 C |
| ATOM | 878 | О | GLY A | 64158.167 | 4.002 | 3.892 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64158.208 | -0.020 | 3.174 | 1.00 | 0.00 H |
| ATOM | 880 | 1HA | GLY A | 64156.457 | 1.574 | 3.492 | 1.00 | 0.00 H |
| ATOM | 881 | 2HA | GLY A | 64157.177 | 2.008 | 5.035 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.674 | 2.647 | 2.168 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.399 | 3.675 | 1.431 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65159.023 | 3.652 | -0.047 | 1.00 | 0.00 C |
| ATOM | 885 | Ο | THR A | 65159.172 | 2.632 | -0.720 | 1.00 | 0.00°O |
| ATOM | 886 | CB | THR A | 65160.908 | 3.476 | 1.589 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.327 | 2.287 | 0.941 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.353 | 3.394 | 3.032 | 1.00 | 0.00 C |

| ATOM | 889 | Н | THR A | 65158.598 | 1.748 | 1.786 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|-------|--------|------|--------|
| ATOM | 890 | НА | THR A | 65159.127 | 4.635 | 1.845 | 1.00 | 0.00 H |
| ATOM | 891 | НВ | THR A | 65161.420 | 4.310 | 1.131 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65160.733 | 1.570 | 1.174 | 1.00 | 0.00 H |
| ATOM | 893 | HG2 | THR A | 65161.703 | 2.395 | 3.245 | 1.00 | 0.00 H |
| ATOM | 894 2 | 2HG2 | THR A | 65160.521 | 3.631 | 3.680 | 1.00 | 0.00 H |
| ATOM | 895 3 | 3HG2 | THR A | 65162.154 | 4.099 | 3.203 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.536 | 4.784 | -0.546 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.138 | 4.894 | -1.945 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.106 | 5.785 | -2.717 | 1.00 | 0.00 C |
| ATOM | 899 | 0 | PHE A | 66159.243 | 6.971 | -2.422 | 1.00 | 0.00 O |
| ATOM | 900 | СВ | PHE A | 66156.718 | 5.452 | -2.051 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.051 | 5.152 | -3.362 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.567 | 6.177 | -4.159 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.908 | 3.844 | -3.798 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66154.953 | 5.903 | -5.367 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.294 | 3.564 | -5.004 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.816 | 4.596 | -5.790 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.441 | 5.563 | 0.040 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66158.159 | 3.904 | -2.374 | 1.00 | 0.00 H |
| ATOM | 909 | IНВ | PHE A | 66156.112 | 5.028 | -1.265 | 1.00 | 0.00 H |
| ATOM | 910 2 | 2HB | PHE A | 66156.752 | 6.526 | -1.931 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66155.674 | 7.200 | -3.829 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.282 | 3.037 | -3.185 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66154.579 | 6.711 | -5.978 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.189 | 2.541 | -5.333 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.337 | 4.379 | -6.732 | 1.00 | 0.00 H |

| ATOM | 916 | N | ARG A | 67159.776 | 5.204 | -3.706 | 1.00 | 0.00 N |
|------|-----|--------|-------|-----------|---------|--------|------|--------|
| ATOM | 917 | CA | ARG A | 67160.732 | 5.945 | -4.521 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.860 | 6.505 | -3.662 | 1.00 | 0.00 C |
| ATOM | 919 | O | ARG A | 67162.359 | 7.602 | -3.913 | 1.00 | 0.00 Q |
| ATOM | 920 | СВ | ARG A | 67160.026 | 7.082 | -5.263 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67158.955 | 6.606 | -6.229 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67158.909 | 7.468 | -7.481 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67160.062 | 7.236 | -8.347 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67160.434 | 8.061 | -9.323 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67159.746 | 9.171 | -9.562 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67161.496 | 7.775 - | 10.064 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.624 | 4.254 | -3.893 | 1.00 | 0.00 H |
| ATOM | 928 | HA | ARG A | 67161.150 | 5.261 | -5.244 | 1.00 | 0.00 H |
| ATOM | 929 | 1HB | ARG A | 67159.564 | 7.736 | -4.539 | 1.00 | 0.00 H |
| ATOM | 930 | 2HB | ARG A | 67160.762 | 7.642 | -5.822 | 1.00 | 0.00 H |
| ATOM | 931 | 1HG | ARG A | 67159.166 | 5.587 | -6.514 | 1.00 | 0.00 H |
| ATOM | 932 | 2HG | ARG A | 67157.994 | 6.651 | -5.736 | 1.00 | 0.00 H |
| ATOM | 933 | 1HD | ARG A | 67158.008 | 7.237 | -8.029 | 1.00 | 0.00 H |
| ATOM | 934 | 2HD | ARG A | 67158.894 | 8.507 | -7.186 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67160.588 | 6.424 | -8.193 | 1.00 | 0.00 H |
| ATOM | 936 | 1HH1 . | ARG A | 67158.944 | 9.393 | -9.007 | 1.00 | 0.00 H |
| ATOM | 937 | 2HH1 . | ARG A | 67160.030 | 9.786 - | 10.297 | 1.00 | 0.00 H |
| ATOM | 938 | 1HH2 . | ARG A | 67162.018 | 6.940 | -9.888 | 1.00 | 0.00 H |
| ATOM | 939 | 2HH2 . | ARG A | 67161.775 | 8.395 - | 10.798 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.258 | 5.744 | -2.648 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.326 | 6.180 | -1.767 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.888 | 7.290 | -0.831 | 1.00 | 0.00 C |
| | | | | | | | | |

| ATOM | 943 | O | GLY A | 68163.699 | 8.118 | -0.417 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|--------|---------|------|--------|
| ATOM | 944 | Н | GLY A | 68161.824 | 4.879 | -2.497 | 1.00 | 0.00 H |
| ATOM | 945 | 1HA | GLY A | 68163.660 | 5.339 | -1.179 | 1.00 | 0.00 H |
| ATOM | 946 | 2HA | GLY A | 68164.150 | 6.537 | -2.368 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.602 | 7.306 | -0.497 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69161.057 | 8.321 | 0.396 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69160.168 | 7.689 | 1.461 | 1.00 | 0.00 C |
| ATOM | 950 | O | THR A | 69159.055 | 7.247 | 1.174 | 1.00 | 0.00 O |
| ATOM | 951 | CB | THR A | 69160.261 | 9.357 | -0.401 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.900 | 9.644 | -1.631 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69160.075 | 10.666 | 0.336 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69161.005 | 6.618 | -0.860 | 1.00 | 0.00 H |
| ATOM | 955 | НА | THR A | 69161.886 | 8.814 | 0.882 | 1.00 | 0.00 H |
| ATOM | 956 | HB | THR A | 69159.281 | 8.955 | -0.614 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.773 | 10.008 | -1.461 | 1.00 | 0.00 H |
| ATOM | 958 | 1HG2 | THR A | 69160.256 | 11.488 | - 0.340 | 1.00 | 0.00 H |
| ATOM | 959 | 2HG2 | THR A | 69160.772 | 10.717 | 1.160 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69159.065 | 10.725 | 0.714 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.666 | 7.649 | 2.693 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.916 | 7.070 | 3.801 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.751 | 7.971 | 4.200 | 1.00 | 0.00 C |
| ATOM | 964 | О | ARG A | 70158.945 | 9.137 | 4.541 | 1.00 | 0.00 O |
| ATOM | 965 | CB | ARG A | 70160.835 | 6.844 | 5.004 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70160.136 | 6.206 | 6.193 | 1.00 | 0.00 C |
| ATOM | 967 | CD | ARG A | 70160.931 | 6.397 | 7.474 | 1.00 | 0.00 C |
| ATOM | 968 | NE | ARG A | 70162.034 | 5.445 | 7.582 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70163.054 | 5.585 | 8.426 | 1.00 | 0.00 C |

| ATOM | 970 | NH1 | ARG A | 70163.116 | 6.635 | 9.235 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 971 | NH2 | ARG A | 70164.015 | 4.673 | 8.459 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.559 | 8.016 | 2.860 | 1.00 | 0.00 H |
| ATOM | 973 | НА | ARG A | 70159.524 | 6.118 | 3.476 | 1.00 | 0.00 H |
| ATOM | 974 | 1HB | ARG A | 70161.649 | 6.200 | 4.704 | 1.00 | 0.00 H |
| ATOM | 975 2 | 2HB | ARG A | 70161.239 | 7.796 | 5.318 | 1.00 | 0.00 H |
| ATOM | 976 | HG | ARG A | 70159.164 | 6.660 | 6.312 | 1.00 | 0.00 H |
| ATOM | 977 2 | 2HG | ARG A | 70160.020 | 5.149 | 6.005 | 1.00 | 0.00 H |
| ATOM | 978 | IHD | ARG A | 70161.331 | 7.400 | 7.489 | 1.00 | 0.00 H |
| ATOM | 979 2 | 2HD | ARG A | 70160.268 | 6.263 | 8.317 | 1.00 | 0.00 H |
| ATOM | 980 | HE | ARG A | 70162.013 | 4.661 | 6.995 | 1.00 | 0.00 H |
| ATOM | 981 | IHH1 | ARG A | 70162.394 | 7.327 | 9.215 | 1.00 | 0.00 H |
| ATOM | 982 2 | 2HH1 | ARG A | 70163.885 | 6.734 | 9.866 | 1.00 | 0.00 H |
| ATOM | 983 1 | HH2 | ARG A | 70163.974 | 3.880 | 7.851 | 1.00 | 0.00 H |
| ATOM | 984 2 | 2HH2 | ARG A | 70164.782 | 4.778 | 9.092 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.543 | 7.421 | 4.154 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71156.346 | 8.176 | 4.510 | 1.00 | 0.00 C |
| ATOM | 987 | C | TYR A | 71155.852 | 7.788 | 5.900 | 1.00 | 0.00 C |
| ATOM | 988 | O | TYR A | 71155.446 | 8.644 | 6.686 | 1.00 | 0.00 O |
| ATOM | 989 | CB | TYR A | 71155.242 | 7.936 | 3.479 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.536 | 8.538 | 2.124 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71156.048 | 9.825 | 2.011 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.304 | 7.820 | 0.958 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71156.318 | 10.379 | 0.773 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.572 | 8.367 | -0.283 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71156.079 | 9.647 | -0.369 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71156.347 | 10.193 | -1.603 | 1.00 | 0.00 O |

| ATOM | 997 | Н | TYR A | 71157.452 | 6.487 | 3.874 | 1.00 | 0.00 H | |
|------|--------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 998 | НА | TYR A | 71156.604 | 9.224 | 4.511 | 1.00 | 0.00 H | |
| ATOM | 999 1 | НВ | TYR A | 71155.106 | 6.873 | 3.346 | 1.00 | 0.00 H | |
| ATOM | 1000 2 | HB | TYR A | 71154.321 | 8.368 | 3.842 | 1.00 | 0.00 H | |
| ATOM | 1001 | HD1 | TYR A | 71156.234 | 10.397 | 2.908 | 1.00 | 0.00 H | |
| ATOM | 1002 | HD2 | TYR A | 71154.906 | 6.819 | 1.029 | 1.00 | 0.00 H | |
| ATOM | 1003 | HE1 | TYR A | 71156.716 | 11.381 | 0.706 | 1.00 | 0.00 H | |
| ATOM | 1004 | HE2 | TYR A | 71155.384 | 7.793 | -1.178 | 1.00 | 0.00 H | |
| ATOM | 1005 | НН | TYR A | 71157.236 | 9.952 | -1.874 | 1.00 | 0.00 H | |
| ATOM | 1006 | N | PHE A | 72155.891 | 6.494 | 6.197 | 1.00 | 0.00 N | |
| ATOM | 1007 | CA | PHE A | 72155.448 | 5.993 | 7.492 | 1.00 | 0.00 C | |
| ATOM | 1008 | C | PHE A | 72156.433 | 4.968 | 8.045 | 1.00 | 0.00 C | |
| ATOM | 1009 | O | PHE A | 72157.368 | 4.556 | 7.358 | 1.00 | 0.00 O | |
| ATOM | 1010 | CB | PHE A | 72154.057 | 5.368 | 7.373 | 1.00 | 0.00 C | |
| ATOM | 1011 | CG | PHE A | 72153.981 | 4.262 | 6.359 | 1.00 | 0.00 C | |
| ATOM | 1012 | CD1 | PHE A | 72154.205 | 2.946 | 6.733 | 1.00 | 0.00 C | |
| ATOM | 1013 | CD2 | PHE A | 72153.686 | 4.538 | 5.034 | 1.00 | 0.00 C | |
| ATOM | 1014 | CE1 | PHE A | 72154.135 | 1.926 | 5.802 | 1.00 | 0.00 C | |
| ATOM | 1015 | CE2 | PHE A | 72153.616 | 3.522 | 4.099 | 1.00 | 0.00 C | |
| ATOM | 1016 | CZ | PHE A | 72153.841 | 2.214 | 4.484 | 1.00 | 0.00 C | |
| ATOM | 1017 | Н | PHE A | 72156.226 | 5.859 | 5.528 | 1.00 | 0.00 H | |
| ATOM | 1018 | НА | PHE A | 72155.399 | 6.831 | 8.172 | 1.00 | 0.00 H | |
| ATOM | 1019 1 | НВ | PHE A | 72153.769 | 4.961 | 8.330 | 1.00 | 0.00 H | |
| ATOM | 1020 2 | HB | PHE A | 72153.350 | 6.133 | 7.084 | 1.00 | 0.00 H | |
| ATOM | 1021 | HD1 | PHE A | 72154.434 | 2.719 | 7.763 | 1.00 | 0.00 H | |
| ATOM | 1022 | HD2 | PHE A | 72153.511 | 5.560 | 4.731 | 1.00 | 0.00 H | |
| ATOM | 1023 | HEI | PHE A | 72154.311 | 0.905 | 6.106 | 1.00 | 0.00 H | |

| ATOM | 1024 | HE2 | PHE A | 72153.386 | 3.751 | 3.069 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1025 | HZ | PHE A | 72153.786 | 1.419 | 3.756 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73156.216 | 4.559 | 9.291 | 1.00 | 0.00 N |
| ATOM | 1027 | CA | THR A | 73157.085 | 3.581 | 9.937 | 1.00 | 0.00 C |
| ATOM | 1028 | C | THR A | 73156.374 | 2.242 | 10.094 | 1.00 | 0.00 C |
| ATOM | 1029 | О | THR A | 73155.396 | 2.129 | 10.834 | 1.00 | 0.00 O |
| ATOM | 1030 | СВ | THR A | 73157.538 | 4.094 | 11.304 | 1.00 | 0.00 C |
| ATOM | 1031 | OG1 | THR A | 73157.838 | 5.477 | 11.247 | 1.00 | 0.00 O |
| ATOM | 1032 | CG2 | THR A | 73158.761 | 3.380 | 11.837 | 1.00 | 0.00 C |
| ATOM | 1033 | H | THR A | 73155.455 | 4.923 | 9.789 | 1.00 | 0.00 H |
| ATOM | 1034 | НА | THR A | 73157.952 | 3.443 | 9.309 | 1.00 | 0.00 H |
| ATOM | 1035 | НВ | THR A | 73156.736 | 3.951 | 12.015 | 1.00 | 0.00 H |
| ATOM | 1036 | HG1 | THR A | 73157.472 | 5.918 | 12.018 | 1.00 | 0.00 H |
| ATOM | 1037 | 1HG2 | THR A | 73159.373 | 4.077 | 12.389 | 1.00 | 0.00 H |
| ATOM | 1038 | 2HG2 | THR A | 73159.331 | 2.978 | 11.011 | 1.00 | 0.00 H |
| ATOM | 1039 | 3HG2 | THR A | 73158.454 | 2.575 | 12.487 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYS A | 74156.871 | 1.227 | 9.394 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74156.282 | -0.106 | 9.455 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74157.366 | -1.179 | 9.459 | 1.00 | 0.00 C |
| ATOM | 1043 | O | CYS A | 74158.558 | -0.871 | 9.475 | 1.00 | 0.00 O |
| ATOM | 1044 | СВ | CYS A | 74155.336 | -0.324 | 8.272 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYS A | 74153.626 | 0.165 | 8.594 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYSA | 74157.652 | 1.380 | 8.821 | 1.00 | 0.00 H |
| ATOM | 1047 | HA | CYS A | 74155.718 | -0.177 | 10.373 | 1.00 | 0.00 H |
| ATOM | 1048 | 1HB | CYS A | 74155.688 | 0.251 | 7.429 | 1.00 | 0.00 H |
| ATOM | 1049 | 2HB | CYS A | 74155.336 | -1.372 | 8.011 | 1.00 | 0.00 H |
| ATOM | 1050 | HG | CYS A | 74153.519 | 0.260 | 9.543 | 1.00 | 0.00 H |

| ATOM | 1051 | N | ALA A | 75156.944 | -2.438 | 9.446 | 1.00 | 0.00 N |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1052 | CA | ALAA | 75157.878 | -3.557 | 9.448 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75158.504 | -3.753 | 8.071 | 1.00 | 0.00 C |
| ATOM | 1054 | O | ALA A | 75158.021 | -3.212 | 7.077 | 1.00 | 0.00 O |
| ATOM | 1055 | СВ | ALA A | 75157.177 | -4.830 | 9.897 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALA A | 75155.981 | -2.620 | 9.434 | 1.00 | 0.00 H |
| ATOM | 1057 | НА | ALA A | 75158.661 | -3.336 | 10.159 | 1.00 | 0.00 H |
| ATOM | 1058 | lНВ | ALA A | 75156.438 | -4.588 | 10.647 | 1.00 | 0.00 H |
| ATOM | 1059 2 | 2HB | ALA A | 75157.902 | -5.513 | 10.314 | 1.00 | 0.00 H |
| ATOM | 1060 3 | ЗНВ | ALA A | 75156.692 | -5.292 | 9.049 | 1.00 | 0.00 H |
| ATOM | 1061 | N | LEU A | 76159.581 | -4.530 | 8.021 | 1.00 | 0.00 N |
| ATOM | 1062 | CA | LEU A | 76160.273 | -4.798 | 6.765 | 1.00 | 0.00 C |
| ATOM | 1063 | C | LEU A | 76159.514 | -5.828 | 5.935 | 1.00 | 0.00 C |
| ATOM | 1064 | O | LEU A | 76158.956 | -6.784 | 6.473 | 1.00 | 0.00 O |
| ATOM | 1065 | CB | LEU A | 76161.695 | -5.292 | 7.037 | 1.00 | 0.00 C |
| ATOM | 1066 | CG | LEU A | 76162.712 | -4.195 | 7.352 | 1.00 | 0.00 C |
| ATOM | 1067 | CD1 | LEU A | 76163.770 | -4.708 | 8.317 | 1.00 | 0.00 C |
| ATOM | 1068 | CD2 | LEU A | 76163.358 | -3.686 | 6.072 | 1.00 | 0.00 C |
| ATOM | 1069 | Н | LEU A | 76159.919 | -4.933 | 8.848 | 1.00 | 0.00 H |
| ATOM | 1070 | НА | LEU A | 76160.323 | -3.872 | 6.212 | 1.00 | 0.00 H |
| ATOM | 1071 | IНВ | LEU A | 76161.661 | -5.975 | 7.874 | 1.00 | 0.00 H |
| ATOM | 1072 2 | 2HB | LEU A | 76162.038 | -5.832 | 6.168 | 1.00 | 0.00 H |
| ATOM | 1073 | HG | LEU A | 76162.204 | -3.366 | 7.824 | 1.00 | 0.00 H |
| ATOM | 1074 | HD1 | LEU A | 76164.717 | -4.240 | 8.096 | 1.00 | 0.00 H |
| ATOM | 1075 2 | 2HD1 | LEU A | 76163.865 | -5.779 | 8.210 | 1.00 | 0.00 H |
| ATOM | 1076 | BHD1 | LEU A | 76163.478 | -4.472 | 9.330 | 1.00 | 0.00 H |
| ATOM | 1077 | HD2 | LEU A | 76162.688 | -3.851 | 5.241 | 1.00 | 0.00 H |

| ATOM | 1078 2HD | 2 LEU A | 76164.282 | -4.216 | 5.899 | 1.00 | 0.00 H |
|------|----------|---------|-----------|---------|-------|------|--------|
| ATOM | 1079 3HD | 2 LEU A | 76163.562 | -2.630 | 6.166 | 1.00 | 0.00 H |
| ATOM | 1080 N | LYS A | 77159.498 | -5.627 | 4.621 | 1.00 | 0.00 N |
| ATOM | 1081 CA | LYS A | 77158.807 | -6.538 | 3.716 | 1.00 | 0.00 C |
| ATOM | 1082 C | LYS A | 77157.311 | -6.563 | 4.005 | 1.00 | 0.00 C |
| ATOM | 1083 O | LYS A | 77156.676 | -7.618 | 3.962 | 1.00 | 0.00 O |
| ATOM | 1084 CB | LYS A | 77159.387 | -7.948 | 3.836 | 1.00 | 0.00 C |
| ATOM | 1085 CG | LYS A | 77160.907 | -7.984 | 3.832 | 1.00 | 0.00 C |
| ATOM | 1086 CD | LYS A | 77161.469 | -7.583 | 2.478 | 1.00 | 0.00 C |
| ATOM | 1087 CE | LYS A | 77162.944 | -7.228 | 2.570 | 1.00 | 0.00 C |
| ATOM | 1088 NZ | LYS A | 77163.150 | -5.792 | 2.908 | 1.00 | 0.00 N |
| ATOM | 1089 H | LYS A | 77159.962 | -4.846 | 4.252 | 1.00 | 0.00 H |
| ATOM | 1090 HA | LYSA | 77158.960 | - 6.181 | 2.707 | 1.00 | 0.00 H |
| ATOM | 1091 1HB | LYS A | 77159.041 | -8.389 | 4.760 | 1.00 | 0.00 H |
| ATOM | 1092 2HB | LYS A | 77159.033 | -8.544 | 3.008 | 1.00 | 0.00 H |
| ATOM | 1093 1HG | LYS A | 77161.275 | -7.299 | 4.580 | 1.00 | 0.00 H |
| ATOM | 1094 2HG | LYS A | 77161.235 | -8.987 | 4.066 | 1.00 | 0.00 H |
| ATOM | 1095 1HD | LYS A | 77161.351 | -8.408 | 1.791 | 1.00 | 0.00 H |
| ATOM | 1096 2HD | LYS A | 77160.924 | -6.726 | 2.112 | 1.00 | 0.00 H |
| ATOM | 1097 1HE | LYSA | 77163.401 | -7.837 | 3.337 | 1.00 | 0.00 H |
| ATOM | 1098 2HE | LYS A | 77163.412 | -7.436 | 1.619 | 1.00 | 0.00 H |
| ATOM | 1099 1HZ | LYS A | 77163.311 | -5.241 | 2.041 | 1.00 | 0.00 H |
| ATOM | 1100 2HZ | LYS A | 77163.976 | -5.686 | 3.531 | 1.00 | 0.00 H |
| ATOM | 1101 3HZ | LYS A | 77162.312 | -5.416 | 3.395 | 1.00 | 0.00 H |
| ATOM | 1102 N | LYS A | 78156.750 | -5.395 | 4.301 | 1.00 | 0.00 N |
| ATOM | 1103 CA | LYS A | 78155.326 | -5.284 | 4.597 | 1.00 | 0.00 C |
| ATOM | 1104 C | LYS A | 78154.793 | -3.911 | 4.198 | 1.00 | 0.00 C |

| ATOM | 1105 | О | LYS A | 78153.981 | -3.318 | 4.908 | 1.00 | 0.00 O |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1106 | СВ | LYS A | 78155.074 | -5.529 | 6.086 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.640 | -6.847 | 6.590 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78155.270 | -7.094 | 8.043 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYS A | 78154.151 | -8.116 | 8.169 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78153.312 | -7.875 | 9.376 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.306 | -4.589 | 4.318 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYSA | 78154.809 | -6.038 | 4.024 | 1.00 | 0.00 H |
| ATOM | 1113 1 | НВ | LYS A | 78155.525 | -4.728 | 6.653 | 1.00 | 0.00 H |
| ATOM | 1114 2 | 2HB | LYS A | 78154.009 | -5.529 | 6.264 | 1.00 | 0.00 H |
| ATOM | 1115 1 | HG | LYS A | 78155.244 | -7.651 | 5.986 | 1.00 | 0.00 H |
| ATOM | 1116 2 | HG | LYS A | 78156.716 | -6.823 | 6.500 | 1.00 | 0.00 H |
| ATOM | 1117 1 | HD | LYS A | 78156.139 | -7.463 | 8.568 | 1.00 | 0.00 H |
| ATOM | 1118 2 | HD | LYS A | 78154.947 | -6.164 | 8.487 | 1.00 | 0.00 H |
| ATOM | 1119 1 | HE | LYS A | 78153.526 | -8.055 | 7.291 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYS A | 78154.586 | -9.102 | 8.234 | 1.00 | 0.00 H |
| ATOM | 1121 1 | HZ | LYSA | 78153.289 | -6.859 | 9.599 | 1.00 | 0.00 H |
| ATOM | 1122 2 | 2HZ | LYS A | 78153.703 | -8.388 | 10.191 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYS A | 78152.341 | -8.205 | 9.207 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.255 | -3.413 | 3.056 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.824 | -2.111 | 2.561 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.652 | -2.129 | 1.047 | 1.00 | 0.00 C |
| ATOM | 1127 | O | ALA A | 79155.630 | -2.201 | 0.301 | 1.00 | 0.00 O |
| ATOM | 1128 | CB | ALA A | 79155.822 | -1.036 | 2.968 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79155.901 | -3.932 | 2.534 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.874 | -1.878 | 3.019 | 1.00 | 0.00 H |
| ATOM | 1131 1 | НВ | ALA A | 79155.857 | -0.270 | 2.207 | 1.00 | 0.00 H |

| ATOM | 1132 | 2HB | ALA A | 79156.801 | -1.477 | 3.080 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1133 | 3НВ | ALAA | 79155.515 | -0.597 | 3.906 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.404 | -2.063 | 0.597 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.103 | -2.072 | -0.829 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.276 | -0.851 | -1.218 | 1.00 | 0.00 C |
| ATOM | 1137 | О | LEU A | 80151.095 | -0.756 | -0.884 | 1.00 | 0.00 O |
| ATOM | 1138 | СВ | LEU A | 80152.352 | -3.352 | -1.205 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80151.922 | -3.444 | -2.670 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.135 | -3.587 | -3.575 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEUA | 80150.964 | -4.609 | -2.871 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.667 | -2.007 | 1.240 | 1.00 | 0.00 H |
| ATOM | 1143 | HA | LEU A | 80154.039 | -2.044 | -1.367 | 1.00 | 0.00 H |
| ATOM | 1144 | 1HB | LEU A | 80152.990 | -4.195 | -0.985 | 1.00 | 0.00 H |
| ATOM | 1145 | 2HB | LEU A | 80151.468 | -3.420 | -0.589 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.406 | -2.535 | -2.944 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | LEU A | 80152.858 | -4.131 | -4.466 | 1.00 | 0.00 H |
| ATOM | 1148 | 2HD1 | LEU A | 80153.913 | -4.124 | -3.052 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80153.497 | -2.607 | -3.850 | 1.00 | 0.00 H |
| ATOM | 1150 | 1HD2 | LEU A | 80151.527 | -5.499 | -3.113 | 1.00 | 0.00 H |
| ATOM | 1151 | 2HD2 | LEU A | 80150.285 | -4.382 | -3.679 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80150.403 | -4.774 | -1.963 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.905 | 0.081 | -1.927 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.227 | 1.297 | -2.362 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.405 | 1.041 | -3.622 | 1.00 | 0.00 C |
| ATOM | 1156 | Ο | PHE A | 81151.884 | 0.420 | -4.571 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.246 | 2.408 | -2.621 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.856 | 2.967 | -1.367 | 1.00 | 0.00 C |

| ATOM | 1159 | CD1 | PHE A | 81153.201 | 3.948 | -0.640 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1160 | CD2 | PHE A | 81155.084 | 2.511 | -0.916 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81153.759 | 4.463 | 0.514 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81155.649 | 3.023 | 0.237 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81154.985 | 4.000 | 0.953 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.846 | -0.052 | -2.164 | 1.00 | 0.00 H |
| ATOM | 1165 | НА | PHE A | 81151.563 | 1.607 | -1.570 | 1.00 | 0.00 H |
| ATOM | 1166 | 1HB | PHE A | 81154.045 | 2.019 | -3.234 | 1.00 | 0.00 H |
| ATOM | 1167 | 2HB | PHE A | 81152.759 | 3.218 | -3.145 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81152.243 | 4.310 | -0.982 | 1.00 | 0.00 H |
| ATOM | 1169 | HD2 | PHE A | 81155.604 | 1.747 | -1.476 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81153.240 | 5.228 | 1.072 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81156.607 | 2.659 | 0.578 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.424 | 4.401 | 1.854 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.167 | 1.524 | -3.623 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VAL A | 82149.280 | 1.347 | -4.765 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VALA | 82148.315 | 2.521 | -4.898 | 1.00 | 0.00 C |
| ATOM | 1176 | О | VAL A | 82148.180 | 3.332 | -3.983 | 1.00 | 0.00 O |
| ATOM | 1177 | CB | VAL A | 82148.470 | 0.042 | -4.652 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VAL A | 82149.379 | -1.166 | -4.809 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VALA | 82147.724 | -0.010 | -3.327 | 1.00 | 0.00 C |
| ATOM | 1180 | Н | VAL A | 82149.843 | 2.010 | -2.836 | 1.00 | 0.00 H |
| ATOM | 1181 | НА | VAL A | 82149.889 | 1.292 | -5.656 | 1.00 | 0.00 H |
| ATOM | 1182 | HB | VAL A | 82147.742 | 0.022 | -5.450 | 1.00 | 0.00 H |
| ATOM | 1183 | 1HG1 | VAL A | 82150.018 | -1.028 | -5.668 | 1.00 | 0.00 H |
| ATOM | 1184 | 2HG1 | VAL A | 82148.779 | -2.054 | -4.947 | 1.00 | 0.00 H |
| ATOM | 1185 | 3HG1 | VAL A | 82149.987 | -1.278 | -3.923 | 1.00 | 0.00 H |

| ATOM | 1186 1HG2 | 2 VAL A | 82147.242 | -0.971 | -3.223 | 1.00 | 0.00 H |
|------|-----------|---------|-----------|---------|---------|------|--------|
| ATOM | 1187 2HG2 | 2 VAL A | 82146.979 | 0.771 | -3.303 | 1.00 | 0.00 H |
| ATOM | 1188 3HG2 | 2 VAL A | 82148.422 | 0.131 | -2.515 | 1.00 | 0.00 H |
| ATOM | 1189 N | LYS A | 83147.645 | 2.602 | -6.043 | 1.00 | 0.00 N |
| ATOM | 1190 CA | LYSA | 83146.693 | 3.677 | -6.295 | 1.00 | 0.00 C |
| ATOM | 1191 C | LYS A | 83145.494 | 3.573 | -5.358 | 1.00 | 0.00 C |
| ATOM | 1192 O | LYS A | 83144.809 | 2.552 | -5.318 | 1.00 | 0.00 O |
| ATOM | 1193 CB | LYS A | 83146.223 | 3.638 | -7.751 | 1.00 | 0.00 C |
| ATOM | 1194 CG | LYS A | 83147.353 | 3.770 | -8.758 | 1.00 | 0.00 C |
| ATOM | 1195 CD | LYS A | 83146.881 | 3.453 | -10.168 | 1.00 | 0.00 C |
| ATOM | 1196 CE | LYS A | 83147.739 | 4.151 | -11.212 | 1.00 | 0.00 C |
| ATOM | 1197 NZ | LYS A | 83148.766 | 3.239 | -11.787 | 1.00 | 0.00 N |
| ATOM | 1198 H | LYSA | 83147.796 | 1.924 | -6.735 | 1.00 | 0.00 H |
| ATOM | 1199 HA | LYS A | 83147.196 | 4.615 | -6.114 | 1.00 | 0.00 H |
| ATOM | 1200 1HB | LYS A | 83145.717 | 2.701 | -7.929 | 1.00 | 0.00 H |
| ATOM | 1201 2HB | LYS A | 83145.528 | 4.449 | -7.914 | 1.00 | 0.00 H |
| ATOM | 1202 1HG | LYS A | 83147.728 | 4.782 | -8.734 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.143 | 3.085 | -8.489 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83146.938 | 2.386 | -10.325 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83145.858 | 3.782 | -10.277 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83147.099 | 4.504 - | 12.007 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83148.234 | 4.991 - | 10.749 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83148.971 | 2.466 - | 11.121 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83149.645 | 3.761 - | 11.974 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83148.422 | 2.831 - | 12.680 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.250 | 4.640 | -4.605 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.136 | 4.675 | -3.666 | 1.00 | 0.00 C |

| ATOM | 1213 | C | LEU A | 84142.808 | 4.456 | -4.384 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1214 | О | LEU A | 84141.894 | 3.832 | - 3.844 | 1.00 | 0.00 O |
| ATOM | 1215 | СВ | LEU A | 84144.115 | 6.015 | -2.924 | 1.00 | 0.00 C |
| ATOM | 1216 | CG | LEU A | 84142.921 | 6.222 | -1.990 | 1.00 | 0.00 C |
| ATOM | 1217 | CD1 | LEU A | 84143.105 | 5.434 | -0.703 | 1.00 | 0.00 C |
| ATOM | 1218 | CD2 | LEUA | 84142.732 | 7.702 | -1.689 | 1.00 | 0.00 C |
| ATOM | 1219 | Н | LEU A | 84145.833 | 5.423 | -4.683 | 1.00 | 0.00 H |
| ATOM | 1220 | HA | LEU A | 84144.280 | 3.880 | -2.950 | 1.00 | 0.00 H |
| ATOM | 1221 | 1HB | LEU A | 84145.020 | 6.091 | -2.340 | 1.00 | 0.00 H |
| ATOM | 1222 | 2HB | LEU A | 84144.112 | 6.807 | -3.658 | 1.00 | 0.00 H |
| ATOM | 1223 | HG | LEU A | 84142.025 | 5.863 | -2.476 | 1.00 | 0.00 H |
| ATOM | 1224 | 1HD1 | LEU A | 84142.152 | 5.045 | -0.380 | 1.00 | 0.00 H |
| ATOM | 1225 | 2HD1 | LEU A | 84143.508 | 6.082 | 0.061 | 1.00 | 0.00 H |
| ATOM | 1226 | 3HD1 | LEU A | 84143.789 | 4.616 | -0.878 | 1.00 | 0.00 H |
| ATOM | 1227 | 1HD2 | LEU A | 84142.418 | 8.215 | -2.586 | 1.00 | 0.00 H |
| ATOM | 1228 | 2HD2 | LEU A | 84143.667 | 8.121 | -1.345 | 1.00 | 0.00 H |
| ATOM | 1229 | 3HD2 | LEU A | 84141.981 | 7.821 | -0.924 | 1.00 | 0.00 H |
| ATOM | 1230 | N | LYS A | 85142.708 | 4.971 | -5.606 | 1.00 | 0.00 N |
| ATOM | 1231 | CA | LYS A | 85141.491 | 4.830 | -6.398 | 1.00 | 0.00 C |
| ATOM | 1232 | C | LYS A | 85141.220 | 3.365 | -6.728 | 1.00 | 0.00 C |
| ATOM | 1233 | Ο | LYS A | 85140.075 | 2.975 | -6.956 | 1.00 | 0.00 O |
| ATOM | 1234 | CB | LYS A | 85141.602 | 5.645 | -7.688 | 1.00 | 0.00 C |
| ATOM | 1235 | CG | LYS A | 85142.793 | 5.264 | -8.549 | 1.00 | 0.00 C |
| ATOM | 1236 | CD | LYS A | 85143.264 | 6.434 | -9.398 | 1.00 | 0.00 C |
| ATOM | 1237 | CE | LYS A | 85144.650 | 6.186 | -9.970 | 1.00 | 0.00 C |
| ATOM | 1238 | NZ | LYS A | 85145.138 | 7.346 - | 10.766 | 1.00 | 0.00 N |
| ATOM | 1239 | Н | LYS A | 85143.471 | 5.458 | -5.982 | 1.00 | 0.00 H |

| ATOM | 1240 | HA | LYS A | 85140.670 | 5.213 | -5.811 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 1241 1 | НВ | LYS A | 85140.702 | 5.500 | -8.269 | 1.00 | 0.00 H |
| ATOM | 1242 2 | 2HB | LYS A | 85141.690 | 6.691 | -7.433 | 1.00 | 0.00 H |
| ATOM | 1243 1 | HG | LYSA | 85143.602 | 4.949 | -7.909 | 1.00 | 0.00 H |
| ATOM | 1244 2 | HG | LYS A | 85142.509 | 4.449 | -9.200 | 1.00 | 0.00 H |
| ATOM | 1245 1 | HD | LYS A | 85142.570 | 6.576 - | 10.214 | 1.00 | 0.00 H |
| ATOM | 1246 2 | HD | LYS A | 85143.289 | 7.323 | -8.786 | 1.00 | 0.00 H |
| ATOM | 1247 1 | HE | LYS A | 85145.335 | 6.008 | -9.154 | 1.00 | 0.00 H |
| ATOM | 1248 2 | HE. | LYS A | 85144.613 | 5.314 - | 10.605 | 1.00 | 0.00 H |
| ATOM | 1249 1 | HZ | LYS A | 85146.175 | 7.409 - | 10.708 | 1.00 | 0.00 H |
| ATOM | 1250 2 | .HZ | LYS A | 85144.728 | 8.229 - | 10.401 | 1.00 | 0.00 H |
| ATOM | 1251 3 | HZ | LYS A | 85144.863 | 7.236 - | 11.763 | 1.00 | 0.00 H |
| ATOM | 1252 | N | SER A | 86142.277 | 2.559 | -6.753 | 1.00 | 0.00 N |
| ATOM | 1253 | CA | SER A | 86142.146 | 1.139 | -7.057 | 1.00 | 0.00 C |
| ATOM | 1254 | C | SER-A | 86142.102 | 0.309 | -5.777 | 1.00 | 0.00 C |
| ATOM | 1255 | О | SER A | 86142.605 | -0.814 | -5.737 | 1.00 | 0.00 O |
| ATOM | 1256 | CB | SER A | 86143.308 | 0.676 | -7.938 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.567 | 1.608 | -8.973 | 1.00 | 0.00 O |
| ATOM | 1258 | Н | SER A | 86143.165 | 2.928 | -6.563 | 1.00 | 0.00 H |
| ATOM | 1259 | НА | SER A | 86141.220 | 0.999 | -7.594 | 1.00 | 0.00 H |
| ATOM | 1260 1 | НВ | SER A | 86144.197 | 0.572 | -7.334 | 1.00 | 0.00 H |
| ATOM | 1261 2 | HB | SER A | 86143.062 | -0.278 | -8.382 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86143.066 | 1.365 | -9.755 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.498 | 0.868 | -4.734 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.387 | 0.180 | -3.453 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87139.928 | -0.097 | -3.109 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYS A | 87139.021 | 0.538 | -3.648 | 1.00 | 0.00 O |

| ATOM | 1267 | CB | CYS A | 87142.036 | 1.012 | -2.345 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| | | | | | | | | |
| ATOM | 1268 | SG | CYSA | 87143.843 | 1.034 | -2.401 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYS A | 87141.116 | 1.766 | -4.828 | 1.00 | 0.00 H |
| ATOM | 1270 | HA | CYS A | 87141.910 | -0.761 | -3.537 | 1.00 | 0.00 H |
| ATOM | 1271 | lНВ | CYS A | 87141.693 | 2.032 | -2.424 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.740 | 0.613 | -1.386 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYSA | 87144.122 | 0.522 | -3.164 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.706 | -1.049 | -2.208 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.356 | -1.408 | -1.793 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.267 | -1.531 | -0.272 | 1.00 | 0.00 C |
| ATOM | 1277 | О | ARG A | 88139.211 | -1.983 | 0.376 | 1.00 | 0.00 O |
| ATOM | 1278 | СВ | ARG A | 88137.932 | -2.723 | -2.448 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88137.230 | -2.538 | -3.784 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.718 | -2.566 | -3.627 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.059 | -3.157 | -4.789 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88135.003 | -2.577 | -5.985 | 1.00 | 0.00 C |
| ATOM | 1283 | NH1 | ARG A | 88135.566 | -1.391 | -6.183 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88134.382 | -3.184 | -6.987 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.470 | -1.520 | -1.812 | 1.00 | 0.00 H |
| ATOM | 1286 | HA | ARG A | 88137.691 | -0.623 | -2.119 | 1.00 | 0.00 H |
| ATOM | 1287 | lНВ | ARG A | 88138.810 | -3.332 | -2.608 | 1.00 | 0.00 H |
| ATOM | 1288 2 | 2HB | ARG A | 88137.260 | -3.244 | -1.782 | 1.00 | 0.00 H |
| ATOM | 1289 | lHG | ARG A | 88137.521 | -1.587 | -4.204 | 1.00 | 0.00 H |
| ATOM | 1290 2 | 2HG | ARG A | 88137.529 | -3.335 | -4.449 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88135.471 | -3.146 | -2.750 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.364 | -1.553 | -3.501 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88134.634 | -4.033 | -4.672 | 1.00 | 0.00 H |

| ATOM | 1294 | IHH1 | ARG A | 88136.035 | -0.928 | -5.431 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1295 2 | 2HH1 | ARG A | 88135.520 | -0.961 | -7.084 | 1.00 | 0.00 H |
| ATOM | 1296 | HH2 | ARG A | 88133.956 | -4.077 | -6.844 | 1.00 | 0.00 H |
| ATOM | 1297 2 | 2HH2 | ARG A | 88134.340 | -2.748 | -7.887 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.126 | -1.131 | 0.319 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89136.924 | -1.201 | 1.769 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.168 | -2.603 | 2.320 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.530 | -3.566 | 1.898 | 1.00 | 0.00 O |
| ATOM | 1302 | СВ | PRO A | 89135.455 | -0.807 | 1.948 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.126 | -0.003 | 0.740 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89135.949 | -0.581 | -0.377 | 1.00 | 0.00 C |
| ATOM | 1305 | НА | PRO A | 89137.555 | -0.497 | 2.291 | 1.00 | 0.00 H |
| ATOM | 1306 1 | IHB | PRO A | 89134.846 | -1.698 | 2.009 | 1.00 | 0.00 H |
| ATOM | 1307 2 | 2HB | PRO A | 89135.343 | -0.225 | 2.851 | 1.00 | 0.00 H |
| ATOM | 1308 1 | IHG | PRO A | 89134.074 | -0.091 | 0.515 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89135.390 | 1.031 | 0.903 | 1.00 | 0.00 H |
| ATOM | 1310 1 | IHD | PRO A | 89135.401 | -1.361 | -0.886 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89136.239 | 0.195 | -1.072 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASPA | 90138.095 | -2.707 | 3.267 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASPA | 90138.422 | -3.991 | 3.877 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.795 | -4.110 | 5.262 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASPA | 90138.296 | -3.540 | 6.232 | 1.00 | 0.00 O |
| ATOM | 1316 | CB | ASP A | 90139.940 | -4.160 | 3.977 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90140.365 | -5.614 | 3.896 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASPA | 90139.547 | -6.492 | 4.244 | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | ASPA | 90141.516 | -5.873 | 3.485 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.570 | -1.902 | 3.563 | 1.00 | 0.00 H |

| ATOM | 1321 | HA | ASPA | 90138.023 | -4.769 | 3.245 | 1.00 | 0.00 H | |
|------|--------|------------|-------|-----------|---------|-------|------|--------|--|
| ATOM | 1322 1 | НВ | ASPA | 90140.410 | -3.622 | 3.168 | 1.00 | 0.00 H | |
| ATOM | 1323 2 | 2HB | ASPA | 90140.279 | -3.756 | 4.919 | 1.00 | 0.00 H | |
| ATOM | 1324 | N | SER A | 91136.695 | -4.850 | 5.346 | 1.00 | 0.00 N | |
| ATOM | 1325 | CA | SER A | 91135.997 | -5.042 | 6.613 | 1.00 | 0.00 C | |
| ATOM | 1326 | C . | SER A | 91136.378 | -6.376 | 7.247 | 1.00 | 0.00 C | |
| ATOM | 1327 | O | SER A | 91135.575 | -6.993 | 7.947 | 1.00 | 0.00 O | |
| ATOM | 1328 | СВ | SER A | 91134.485 | -4.978 | 6.401 | 1.00 | 0.00 C | |
| ATOM | 1329 | OG | SER A | 91133.828 | -4.483 | 7.554 | 1.00 | 0.00 O | |
| ATOM | 1330 | Н | SER A | 91136.343 | -5.278 | 4.537 | 1.00 | 0.00 H | |
| ATOM | 1331 | НА | SER A | 91136.293 | -4.243 | 7.277 | 1.00 | 0.00 H | |
| ATOM | 1332 1 | НВ | SER A | 91134.267 | -4.326 | 5.569 | 1.00 | 0.00 H | |
| ATOM | 1333 2 | 2HB | SER A | 91134.112 | -5.970 | 6.187 | 1.00 | 0.00 H | |
| ATOM | 1334 | HG | SER A | 91133.100 | -5.065 | 7.784 | 1.00 | 0.00 H | |
| ATOM | 1335 | N | ARG A | 92137.608 | -6.815 | 6.999 | 1.00 | 0.00 N | |
| ATOM | 1336 | CA | ARG A | 92138.093 | -8.076 | 7.546 | 1.00 | 0.00 C | |
| ATOM | 1337 | C | ARG A | 92138.164 | -8.018 | 9.069 | 1.00 | 0.00 C | |
| ATOM | 1338 | O | ARG A | 92137.993 | -9.030 | 9.748 | 1.00 | 0.00 O | |
| ATOM | 1339 | СВ | ARG A | 92139.471 | -8.409 | 6.972 | 1.00 | 0.00 C | |
| ATOM | 1340 | CG | ARG A | 92139.416 | -9.230 | 5.695 | 1.00 | 0.00 C | |
| ATOM | 1341 | CD | ARG A | 92139.022 | -10.671 | 5.976 | 1.00 | 0.00 C | |
| ATOM | 1342 | NE | ARG A | 92137.589 | -10.891 | 5.797 | 1.00 | 0.00 N | |
| ATOM | 1343 | CZ | ARG A | 92137.005 | -11.048 | 4.612 | 1.00 | 0.00 C | |
| ATOM | 1344 | NHI | ARG A | 92137.727 | -11.011 | 3.498 | 1.00 | 0.00 N | |
| ATOM | 1345 | NH2 | ARG A | 92135.696 | -11.243 | 4.538 | 1.00 | 0.00 N | |
| ATOM | 1346 | Н | ARG A | 92138.202 | - 6.278 | 6.434 | 1.00 | 0.00 H | |
| ATOM | 1347 | НА | ARG A | 92137.398 | -8.851 | 7.260 | 1.00 | 0.00 H | |
| | | | | | | | | | |

| ATOM | 1348 | lНВ | ARG A | 92139.992 | -7.486 | 6.760 | 1.00 | 0.00 H |
|------|--------|--------|-------|-------------|---------|--------|------|--------|
| ATOM | 1349 | 2HB | ARG A | 92140.030 | -8.966 | 7.709 | 1.00 | 0.00 H |
| ATOM | 1350 | 1HG | ARG A | 92138.688 | -8.792 | 5.028 | 1.00 | 0.00 H |
| ATOM | 1351 2 | 2HG | ARG A | 92140.390 | -9.216 | 5.227 | 1.00 | 0.00 H |
| ATOM | 1352 | 1HD | ARG A | 92139.562 | -11.318 | 5.300 | 1.00 | 0.00 H |
| ATOM | 1353 | 2HD | ARG A | 92139.290 | -10.912 | 6.994 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92137.032 | -10.923 | 6.603 | 1.00 | 0.00 H |
| ATOM | 1355 | 1HH1. | ARG A | 92138.714 - | 10.864 | 3.546 | 1.00 | 0.00 H |
| ATOM | 1356 | 2HH1. | ARG A | 92137.282 - | 11.130 | 2.611 | 1.00 | 0.00 H |
| ATOM | 1357 | 1HH2 | ARG A | 92135.147 - | 11.273 | 5.374 | 1.00 | 0.00 H |
| ATOM | 1358 2 | 2HH2 . | ARG A | 92135.256 - | 11.362 | 3.648 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93138.419 | -6.825 | 9.599 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93138.513 | -6.636 | 11.042 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93137.293 | -5.889 | 11.574 | 1.00 | 0.00 C |
| ATOM | 1362 | О | PHE A | 93137.385 | -5.153 | 12.557 | 1.00 | 0.00 O |
| ATOM | 1363 | CB | PHE A | 93139.788 | -5.868 | 11.393 | 1.00 | 0.00 C |
| ATOM | 1364 | CG | PHE A | 93141.045 | -6.662 | 11.179 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93141.370 | -7.144 | 9.921 | 1.00 | 0.00 C |
| ATOM | 1366 | CD2 | PHE A | 93141.902 | -6.927 | 12.236 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93142.526 | -7.875 | 9.721 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93143.059 | -7.658 | 12.041 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ. | PHE A | 93143.371 | -8.132 | 10.782 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93138.546 | -6.056 | 9.006 | 1.00 | 0.00 H |
| ATOM | 1371 | HA | PHE A | 93138.552 | -7.611 | 11.502 | 1.00 | 0.00 H |
| ATOM | 1372 | 1HB | PHE A | 93139.848 | -4.982 | 10.780 | 1.00 | 0.00 H |
| ATOM | 1373 2 | 2HB | PHE A | 93139.751 | -5.578 | 12.433 | 1.00 | 0.00 H |
| ATOM | 1374 | HD1 | PHE A | 93140.710 | -6.943 | 9.090 | 1.00 | 0.00 H |

| ATOM | 1375 | HD2 | PHE A | 93141.658 | -6.557 | 13.220 | 1.00 | 0.00 H | |
|------|--------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 1376 | HE1 | PHE A | 93142.768 | -8.246 | 8.735 | 1.00 | 0.00 H | |
| ATOM | 1377 | HE2 | PHE A | 93143.718 | -7.857 | 12.873 | 1.00 | 0.00 H | |
| ATOM | 1378 | HZ | PHE A | 93144.275 | -8.704 | 10.629 | 1.00 | 0.00 H | |
| ATOM | 1379 | N | ALA A | 94136.153 | -6.084 | 10.920 | 1.00 | 0.00 N | |
| ATOM | 1380 | CA | ALA A | 94134.917 | -5.429 | 11.329 | 1.00 | 0.00 C | |
| ATOM | 1381 | C | ALA A | 94134.552 | -5.791 | 12.766 | 1.00 | 0.00 C | |
| ATOM | 1382 | O | ALA A | 94134.390 | -6.965 | 13.099 | 1.00 | 0.00 O | |
| ATOM | 1383 | CB | ALAA | 94133.784 | -5.803 | 10.384 | 1.00 | 0.00 C | |
| ATOM | 1384 | Н | ALA A | 94136.142 | -6.682 | 10.143 | 1.00 | 0.00 H | |
| ATOM | 1385 | НА | ALA A | 94135.069 | -4.361 | 11.267 | 1.00 | 0.00 H | |
| ATOM | 1386 1 | HB | ALA A | 94134.071 | -6.665 | 9.802 | 1.00 | 0.00 H | |
| ATOM | 1387 2 | HB | ALA A | 94133.579 | -4.974 | 9.722 | 1.00 | 0.00 H | |
| ATOM | 1388 3 | НВ | ALA A | 94132.897 | -6.034 | 10.956 | 1.00 | 0.00 H | |
| ATOM | 1389 | N | SER A | 95134.426 | -4.775 | 13.614 | 1.00 | 0.00 N | |
| ATOM | 1390 | CA | SER A | 95134.082 | -4.987 | 15.014 | 1.00 | 0.00 C | |
| ATOM | 1391 | C | SER A | 95132.642 | -4.567 | 15.290 | 1.00 | 0.00 C | |
| ATOM | 1392 | 0 | SER A | 95132.089 | -3.714 | 14.596 | 1.00 | 0.00 O | |
| ATOM | 1393 | CB | SER A | 95135.036 | -4.205 | 15.920 | 1.00 | 0.00 C | |
| ATOM | 1394 | OG | SER A | 95136.145 | -5.000 | 16.300 | 1.00 | 0.00 O | |
| ATOM | 1395 | Н | SER A | 95134.568 | -3.861 | 13.289 | 1.00 | 0.00 H | |
| ATOM | 1396 | НА | SER A | 95134.184 | -6.041 | 15.225 | 1.00 | 0.00 H | |
| ATOM | 1397 1 | HB | SER A | 95135.397 | -3.335 | 15.392 | 1.00 | 0.00 H | |
| ATOM | 1398 2 | НВ | SER A | 95134.509 | -3.893 | 16.809 | 1.00 | 0.00 H | |
| ATOM | 1399 | HG | SER A | 95136.483 | -5.467 | 15.533 | 1.00 | 0.00 H | |
| ATOM | 1400 | N | LEU A | 96132.039 | -5.172 | 16.308 | 1.00 | 0.00 N | |
| ATOM | 1401 | CA | LEU A | 96130.663 | -4.861 | 16.676 | 1.00 | 0.00 C | |

| ATOM | 1402 | C | LEU A | 96130.285 | -5.533 | 17.992 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1403 | О | LEU A | 96129.953 | -6.718 | 18.023 | 1.00 | 0.00 O |
| ATOM | 1404 | СВ | LEU A | 96129.704 | -5.307 | 15.570 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96128.495 | -4.395 | 15.355 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96127.882 | -4.636 | 13.984 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96127.462 | -4.613 | 16.450 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96132.531 | -5.845 | 16.825 | 1.00 | 0.00 H |
| ATOM | 1409 | НА | LEU A | 96130.586 | -3.792 | 16.797 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96130.258 | -5.361 | 14.644 | 1.00 | 0.00 H |
| ATOM | 1411 | 2HB | LEU A | 96129.341 | -6.295 | 15.812 | 1.00 | 0.00 H |
| ATOM | 1412 | HG | LEU A | 96128.817 | -3.364 | 15.399 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96128.625 | -5.066 | 13.328 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96127.538 | -3.698 | 13.573 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96127.048 | -5.315 | 14.077 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96127.130 | -5.641 | 16.431 | 1.00 | 0.00 H |
| ATOM | 1417 | 2HD2 | LEU A | 96126.618 | -3.960 | 16.283 | 1.00 | 0.00 H |
| ATOM | 1418 | 3HD2 | LEU A | 96127.903 | -4.395 | 17.410 | 1.00 | 0.00 H |
| ATOM | 1419 | N | GLN A | 97130.339 | -4.769 | 19.079 | 1.00 | 0.00 N |
| ATOM | 1420 | CA | GLN A | 97130.002 | -5.290 | 20.398 | 1.00 | 0.00 C |
| ATOM | 1421 | C | GLN A | 97130.929 | -6.442 | 20.781 | 1.00 | 0.00 C |
| ATOM | 1422 | Ο | GLN A | 97131.595 | -7.024 | 19.925 | 1.00 | 0.00 O |
| ATOM | 1423 | CB | GLN A | 97128.547 | -5.759 | 20.427 | 1.00 | 0.00 C |
| ATOM | 1424 | CG | GLN A | 97127.566 | -4.676 | 20.847 | 1.00 | 0.00 C |
| ATOM | 1425 | CD | GLN A | 97126.204 | -4.841 | 20.203 | 1.00 | 0.00 C |
| ATOM | 1426 | OE1 | GLN A | 97126.054 | -4.681 | 18.992 | 1.00 | 0.00 O |
| ATOM | 1427 | NE2 | GLN A | 97125.201 | -5.162 | 21.013 | 1.00 | 0.00 N |
| ATOM | 1428 | Н | GLN A | 97130.611 | -3.831 | 18.990 | 1.00 | 0.00 H |

| ATOM | 1429 | НА | GLN A | 97130.127 | -4.490 | 21.112 | 1.00 | 0.00 H |
|------|--------|------|-------|-------------|---------|--------|------|--------|
| ATOM | 1430 | lНВ | GLN A | 97128.271 | -6.100 | 19.441 | 1.00 | 0.00 H |
| ATOM | 1431 2 | 2HB | GLN A | 97128.459 | -6.583 | 21.121 | 1.00 | 0.00 H |
| ATOM | 1432 | HG | GLN A | 97127.447 | -4.713 | 21.920 | 1.00 | 0.00 H |
| ATOM | 1433 2 | 2HG | GLN A | 97127.970 | -3.714 | 20.564 | 1.00 | 0.00 H |
| ATOM | 1434 | HE2 | GLN A | 97125.395 | -5.274 | 21.967 | 1.00 | 0.00 H |
| ATOM | 1435 2 | 2HE2 | GLN A | 97124.310 | -5.275 | 20.622 | 1.00 | 0.00 H |
| ATOM | 1436 | N | PRO A | 98130.983 | -6.785 | 22.080 | 1.00 | 0.00 N |
| ATOM | 1437 | CA | PRO A | 98131.833 | -7.874 | 22.573 | 1.00 | 0.00 C |
| ATOM | 1438 | C | PRO A | 98131.336 | -9.245 | 22.127 | 1.00 | 0.00 C |
| ATOM | 1439 | O | PRO A | 98130.179 | -9.599 | 22.350 | 1.00 | 0.00 O |
| ATOM | 1440 | CB | PRO A | 98131.737 | -7.739 | 24.095 | 1.00 | 0.00 C |
| ATOM | 1441 | CG | PRO A | 98130.430 | -7.067 | 24.333 | 1.00 | 0.00 C |
| ATOM | 1442 | CD | PRO A | 98130.221 | -6.142 | 23.166 | 1.00 | 0.00 C |
| ATOM | 1443 | НА | PRO A | 98132.859 | -7.746 | 22.261 | 1.00 | 0.00 H |
| ATOM | 1444 | HB | PRO A | 98131.767 | -8.720 | 24.548 | 1.00 | 0.00 H |
| ATOM | 1445 2 | 2HB | PRO A | 98132.560 | -7.142 | 24.459 | 1.00 | 0.00 H |
| ATOM | 1446 | HG | PRO A | 98129.641 | -7.804 | 24.375 | 1.00 | 0.00 H |
| ATOM | 1447 2 | 2HG | PRO A | 98130.469 | -6.504 | 25.254 | 1.00 | 0.00 H |
| ATOM | 1448 | IHD | PRO A | 98129.171 | -6.080 | 22.917 | 1.00 | 0.00 H |
| ATOM | 1449 2 | 2HD | PRO A | 98130.617 | -5.162 | 23.386 | 1.00 | 0.00 H |
| ATOM | 1450 | N | SER A | 99132.218 - | 10.012 | 21.495 | 1.00 | 0.00 N |
| ATOM | 1451 | CA | SER A | 99131.868 | -11.344 | 21.017 | 1.00 | 0.00 C |
| ATOM | 1452 | C | SER A | 99132.957 - | 12.352 | 21.371 | 1.00 | 0.00 C |
| ATOM | 1453 | О | SER A | 99132.687 - | -13.383 | 21.987 | 1.00 | 0.00 O |
| ATOM | 1454 | CB | SER A | 99131.648 | -11.324 | 19.503 | 1.00 | 0.00 C |
| ATOM | 1455 | OG | SER A | 99132.444 | -10.328 | 18.884 | 1.00 | 0.00 O |

| ATOM | 1456 H | SER A 99133.126 -9.673 | 21.346 | 1.00 | 0.00 H |
|------|----------|--------------------------|--------|------|--------|
| ATOM | 1457 HA | SER A 99130.950 -11.639 | 21.502 | 1.00 | 0.00 H |
| ATOM | 1458 1HB | SER A 99131.914 -12.287 | 19.091 | 1.00 | 0.00 H |
| ATOM | 1459 2HB | SER A 99130.608 -11.119 | 19.296 | 1.00 | 0.00 H |
| ATOM | 1460 HG | SER A 99131.881 -9.611 | 18.582 | 1.00 | 0.00 H |
| ATOM | 1461 N | GLY A 100134.190 -12.047 | 20.978 | 1.00 | 0.00 N |
| ATOM | 1462 CA | GLY A 100135.300 -12.936 | 21.263 | 1.00 | 0.00 C |
| ATOM | 1463 C | GLY A 100135.839 -12.759 | 22.670 | 1.00 | 0.00 C |
| ATOM | 1464 O | GLY A 100135.168 -12.182 | 23.525 | 1.00 | 0.00 O |
| ATOM | 1465 H | GLY A 100134.346 -11.212 | 20.491 | 1.00 | 0.00 H |
| ATOM | 1466 1HA | GLY A 100134.970 -13.957 | 21.141 | 1.00 | 0.00 H |
| ATOM | 1467 2HA | GLY A 100136.095 -12.740 | 20.557 | 1.00 | 0.00 H |
| ATOM | 1468 N | PRO A 101137.062 -13.248 | 22.942 | 1.00 | 0.00 N |
| ATOM | 1469 CA | PRO A 101137.680 -13.133 | 24.267 | 1.00 | 0.00 C |
| ATOM | 1470 C | PRO A 101138.074 -11.697 | 24.600 | 1.00 | 0.00 C |
| ATOM | 1471 O | PRO A 101137.812 -11.210 | 25.698 | 1.00 | 0.00 O |
| ATOM | 1472 CB | PRO A 101138.926 -14.015 | 24.156 | 1.00 | 0.00 C |
| ATOM | 1473 CG | PRO A 101139.252 -14.029 | 22.703 | 1.00 | 0.00 C |
| ATOM | 1474 CD | PRO A 101137.934 -13.949 | 21.982 | 1.00 | 0.00 C |
| ATOM | 1475 HA | PRO A 101137.032 -13.516 | 25.041 | 1.00 | 0.00 H |
| ATOM | 1476 1HB | PRO A 101139.728 -13.586 | 24.738 | 1.00 | 0.00 H |
| ATOM | 1477 2HB | PRO A 101138.701 -15.007 | 24.519 | 1.00 | 0.00 H |
| ATOM | 1478 1HG | PRO A 101139.867 -13.176 | 22.456 | 1.00 | 0.00 H |
| ATOM | 1479 2HG | PRO A 101139.762 -14.947 | 22.450 | 1.00 | 0.00 H |
| ATOM | 1480 1HD | PRO A 101138.037 -13.382 | 21.069 | 1.00 | 0.00 H |
| ATOM | 1481 2HD | PRO A 101137.558 -14.940 | 21.773 | 1.00 | 0.00 H |
| ATOM | 1482 N | SER A 102138.704 -11.024 | 23.642 | 1.00 | 0.00 N |

| ATOM | 1483 | CA | SER A 102139.133 | -9.644 | 23.833 | 1.00 | 0.00 C |
|------|--------|-----|--------------------|---------|--------|------|--------|
| ATOM | 1484 | C | SER A 102139.033 | -8.858 | 22.530 | 1.00 | 0.00 C |
| ATOM | 1485 | O | SER A 102140.038 | -8.608 | 21.865 | 1.00 | 0.00 O |
| ATOM | 1486 | СВ | SER A 102140.569 | -9.602 | 24.359 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102140.652 | -10.160 | 25.659 | 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102138.885 - | 11.467 | 22.786 | 1.00 | 0.00 H |
| ATOM | 1489 | HA | SER A 102138.479 | -9.192 | 24.564 | 1.00 | 0.00 H |
| ATOM | 1490 | 1HB | SER A 102141.209 - | 10.168 | 23.699 | 1.00 | 0.00 H |
| ATOM | 1491 2 | 2HB | SER A 102140.907 | -8.577 | 24.398 | 1.00 | 0.00 H |
| ATOM | 1492 | HG | SER A 102140.083 | -9.667 | 26.256 | 1.00 | 0.00 H |
| ATOM | 1493 | N | SER A 103137.813 | -8.469 | 22.171 | 1.00 | 0.00 N |
| ATOM | 1494 | CA | SER A 103137.575 | -7.710 | 20.947 | 1.00 | 0.00 C |
| ATOM | 1495 | C | SER A 103137.853 | -8.562 | 19.712 | 1.00 | 0.00 C |
| ATOM | 1496 | О | SER A 103136.932 | -8.955 | 18.997 | 1.00 | 0.00 O |
| ATOM | 1497 | СВ | SER A 103138.444 | -6.450 | 20.921 | 1.00 | 0.00 C |
| ATOM | 1498 | OG | SER A 103137.703 | -5.328 | 20.472 | 1.00 | 0.00 O |
| ATOM | 1499 | Н | SER A 103137.051 | -8.699 | 22.744 | 1.00 | 0.00 H |
| ATOM | 1500 | HA | SER A 103136.535 | -7.417 | 20.938 | 1.00 | 0.00 H |
| ATOM | 1501 | IHB | SER A 103138.809 | -6.246 | 21.917 | 1.00 | 0.00 H |
| ATOM | 1502 2 | ΣНВ | SER A 103139.280 | -6.603 | 20.256 | 1.00 | 0.00 H |
| ATOM | 1503 | HG | SER A 103137.240 | -5.554 | 19.662 | 1.00 | 0.00 H |
| ATOM | 1504 | N | GLY A 104139.130 | -8.843 | 19.468 | 1.00 | 0.00 N |
| ATOM | 1505 | CA | GLY A 104139.505 | -9.647 | 18.319 | 1.00 | 0.00 C |
| ATOM | 1506 | C | GLY A 104140.109 | -8.818 | 17.205 | 1.00 | 0.00 C |
| ATOM | 1507 | О | GLY A 104141.142 | -8.158 | 17.448 | 1.00 | 0.00 O |
| ATOM | 1508 | OXT | GLY A 104139.552 | -8.828 | 16.087 | 1.00 | 0.00 O |
| ATOM | 1509 | Н | GLY A 104139.822 | -8.504 | 20.073 | 1.00 | 0.00 H |

ATOM 1510 1HA GLY A 104140.225 -10.388 18.633 1.00 0.00 H
ATOM 1511 2HA GLY A 104138.626 -10.150 17.943 1.00 0.00 H
TER 1512 GLY A 104
ENDMDL

Three-Dimensional Structure Coordinate Table 3

| ATOM 1 | N | GLY A | 1125.212 | 27.334 | -8.433 | 1.00 | 0.00 N |
|----------|-----|-------|----------|--------|---------|------|--------|
| ATOM 2 | CA | GLY A | 1126.127 | 26.226 | -8.041 | 1.00 | 0.00 C |
| ATOM 3 | C | GLY A | 1126.734 | 25.523 | -9.238 | 1.00 | 0.00 C |
| ATOM 4 | Ο | GLY A | 1126.538 | 24.322 | -9.426 | 1.00 | 0.00 O |
| ATOM 5 1 | Н | GLY A | 1125.466 | 27.688 | -9.377 | 1.00 | 0.00 H |
| ATOM 6 2 | Н | GLY A | 1125.283 | 28.114 | -7.751 | 1.00 | 0.00 H |
| ATOM 7 3 | Н | GLY A | 1124.229 | 26.994 | -8.455 | 1.00 | 0.00 H |
| ATOM 8 1 | НА | GLY A | 1126.923 | 26.630 | -7.432 | 1.00 | 0.00 H |
| ATOM 9 2 | НА | GLY A | 1125.572 | 25.506 | -7.457 | 1.00 | 0.00 H |
| ATOM10 | N | SER A | 2127.472 | 26.272 | -10.049 | 1.00 | 0.00 N |
| ATOM11 | CA | SER A | 2128.110 | 25.713 | -11.236 | 1.00 | 0.00 C |
| ATOM12 | C | SER A | 2129.203 | 24.723 | -10.851 | 1.00 | 0.00 C |
| ATOM13 | О | SER A | 2129.120 | 23.536 | -11.169 | 1.00 | 0.00 O |
| ATOM14 | СВ | SER A | 2128.700 | 26.831 | -12.098 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2127.762 | 27.284 | -13.059 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2127.592 | 27.223 | -9.846 | 1.00 | 0.00 H |
| ATOM17 | НА | SER A | 2127.354 | 25.193 | -11.805 | 1.00 | 0.00 H |
| ATOM18 | 1HB | SER A | 2128.978 | 27.662 | -11.466 | 1.00 | 0.00 H |
| ATOM19 | 2HB | SER A | 2129.575 | 26.461 | -12.613 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2127.770 | 28.243 | -13.087 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3130.228 | 25.217 | -10.164 | 1.00 | 0.00 N |

| ATOM22 | CA | SER A | 3131.338 | 24.374 | -9.734 | 1.00 | 0.00 C |
|----------|-----|-------|------------|----------|---------|------|--------|
| ATOM23 | C | SER A | 3130.855 | 23.274 | -8.795 | 1.00 | 0.00 C |
| ATOM24 | O | SER A | 3130.082 | 23.528 | -7.871 | 1.00 | 0.00 O |
| ATOM25 | СВ | SER A | 3132.408 | 25.220 | -9.040 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | · 3132.727 | 26.369 | -9.806 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3130.237 | 26.171 | -9.939 | 1.00 | 0.00 H |
| ATOM28 | НА | SER A | 3131.767 | 23.918 | -10.613 | 1.00 | 0.00 H |
| ATOM29 | IНВ | SER A | 3132.043 | 25.537 | -8.075 | 1.00 | 0.00 H |
| ATOM30 2 | 2HB | SER A | 3133.302 | 24.629 | -8.910 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3132.091 | 27.063 | -9.621 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4131.315 | 22.051 | -9.038 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4130.919 | 20.931 | -8.206 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4130.532 | 19.711 | -9.020 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4129.678 | 19.791 | -9.902 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4131.929 | 21.908 | -9.789 | 1.00 | 0.00 H |
| ATOM37 | НА | GLY A | 4131.742 | 20.670 | -7.557 | 1.00 | 0.00 H |
| ATOM38 2 | 2HA | GLY A | 4130.076 | 21.227 | -7.599 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5131.165 | 18.580 | -8.724 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5130.883 | 17.339 | -9.436 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5129.775 | 16.553 | -8.741 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5129.529 | 16.730 | -7.548 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5132.147 | 16.483 | -9.532 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5132.417 | 15.830 | -8.304 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5131.837 | 18.580 | -8.011 | 1.00 | 0.00 H |
| ATOM46 | HA | SER A | 5130.555 | 17.595 | -10.432 | 1.00 | 0.00 H |
| ATOM47 | lНВ | SER A | 5132.015 | 15.736 - | 10.300 | 1.00 | 0.00 H |
| ATOM48 2 | 2HB | SER A | 5132.987 | 17.113 | -9.784 | 1.00 | 0.00 H |

| ATOM49 | HG | SER A | 5132.762 | 14.951 | -8.477 | 1.00 | 0.00 H |
|--------|-----|-------|----------|----------|----------------|------|--------|
| ATOM50 | N | SER A | 6129.109 | 15.685 | -9.496 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6128.028 | 14.872 | -8.952 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6128.579 | 13.712 | -8.129 | 1.00 | 0.00 C |
| ATOM53 | О | SER A | 6129.231 | 12.814 | -8.662 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6127.146 | 14.337 | -10.081 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6126.755 | 15.378 | -10.960 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6129.352 | 15.588 - | 10.440 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6127.431 | 15.502 | -8.309 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6127.695 | 13.597 - | 10.644 | 1.00 | 0.00 H |
| AŤOM59 | 2HB | SER A | 6126.260 | 13.885 | - 9.661 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6127.535 | 15.778 | -11.351 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7128.313 | 13.737 | -6.827 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7128.790 | 12.683 | -5.952 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7127.664 | 11.816 | -5.421 | 1.00 | 0.00 C |
| ATOM64 | Ο | GLY A | 7127.124 | 12.079 | -4.346 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7127.788 | 14.478 | -6.458 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7129.481 | 12.060 | -6.499 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7129.308 | 13.130 | -5.116 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8127.309 | 10.783 | -6.177 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8126.240 | 9.875 | -5.777 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8126.566 | 9.201 | -4.447 | 1.00 | 0.00 C |
| ATOM71 | Ο. | LEU A | 8125.679 | 8.948 | -3.633 | 1.00 | 0.00 O |
| ATOM72 | CB | LEU A | 8126.012 | 8.815 | -6.857 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8125.799 | 9.364 | -8.267 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8126.357 | 8.401 | -9.305 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8124.323 | 9.626 | -8.520 | 1.00 | 0.00 C |

| ATOM76 H | LEU A | 8127.778 | 10.626 | -7.023 | 1.00 | 0.00 H |
|-------------|-------|-----------|---------|---------|--------|-------------|
| АТОМ77 НА | LEU A | 8125.338 | 10.456 | -5.659 | 1.00 | 0.00 H |
| ATOM78 1HB | LEU A | 8126.869 | 8.158 | -6.872 | 1.00 | 0.00 H |
| ATOM79 2HB | LEU A | 8125.141 | 8.237 | -6.585 | 1.00 | 0.00 H |
| ATOM80 HG | LEU A | 8126.328 | 10.302 | -8.366 | 1.00 | 0.00 H |
| ATOM81 1HD1 | LEU A | 8125.688 | 7.560 | -9.412 | 1.00 | 0.00 H |
| ATOM82 2HD1 | LEU A | 8127.328 | 8.051 | -8.985 | 1.00 | 0.00 H |
| ATOM83 3HD1 | LEU A | 8126.453 | 8.909 - | 10.253 | 1.00 | 0.00 H |
| ATOM84 1HD2 | LEU A | 8124.119 | 9.548 | -9.578 | 1.00 | 0.00 H |
| ATOM85 2HD2 | LEU A | 8124.069 | 10.618 | -8.177 | 1.00 | 0.00 H |
| ATOM86 3HD2 | LEU A | 8123.731 | 8.897 | -7.986 | 1.00 | 0.00 H |
| ATOM87 N | ALA A | 9127.846 | 8.913 | -4.236 | 1.00 | 0.00 N |
| ATOM88 CA | ALA A | 9128.291 | 8.269 | -3.007 | 1.00 | 0.00 C |
| ATOM89 C | ALAA | 9129.810 | 8.310 | -2.884 | 1.00 | 0.00 C |
| ATOM90 O | ALA A | 9130.425 | 7.393 | -2.339 | 1.00 | 0.00 O |
| ATOM91 CB | ALA A | 9127.794 | 6.833 | -2.955 | 1.00 | 0.00 C |
| ATOM92 H | ALA A | 9128.507 | 9.141 | -4.924 | 1.00 | 0.00 H |
| ATOM93 HA | ALA A | 9127.858 | 8.805 | -2.175 | 1.00 | 0.00 H |
| ATOM94 1HB | ALA A | 9128.506 | 6.225 | -2.415 | 1.00 | 0.00 H |
| ATOM95 2HB | ALA A | 9127.686 | 6.452 | -3.960 | 1.00 | 0.00 H |
| ATOM96 3HB | ALA A | 9126.839 | 6.800 | -2.452 | 1.00 | 0.00 H |
| ATOM97 N | MET A | 10130.412 | 9.381 | -3.394 | 1.00 | 0.00 N |
| ATOM98 CA | MET A | 10131.861 | 9.542 | -3.341 | 1.00 | 0.00 C |
| ATOM99 C | MET A | 10132.281 | 10.879 | -3.949 | 1.00 | 0.00 C |
| ATOM 100 | O MI | ETA 1013 | 2.849 1 | 0.924 - | 5.041 | 1.00 0.00 O |
| ATOM 101 | CB M | ETA 1013 | 2.550 | 8.392 | -4.080 | 1.00 0.00 C |
| ATOM 102 | CG M | ETA 1013 | 1.913 | 8.058 | -5.419 | 1.00 0.00 C |

| ATOM | 103 SD | MET A | 10132.616 | 6.579 | -6.173 | 1.00 | 0.00 S |
|------|---------|-------|-----------|--------|--------|------|--------|
| ATOM | 104 CE | MET A | 10132.892 | 7.152 | -7.847 | 1.00 | 0.00 C |
| ATOM | 105 H | MET A | 10129.868 | 10.079 | -3.816 | 1.00 | 0.00 H |
| ATOM | 106 HA | MET A | 10132.159 | 9.522 | -2.304 | 1.00 | 0.00 H |
| ATOM | 107 1HB | MET A | 10133.582 | 8.658 | -4.253 | 1.00 | 0.00 H |
| ATOM | 108 2HB | MET A | 10132.515 | 7.509 | -3.459 | 1.00 | 0.00 H |
| ATOM | 109 1HG | MET A | 10130.855 | 7.900 | -5.270 | 1.00 | 0.00 H |
| ATOM | 110 2HG | MET A | 10132.060 | 8.892 | -6.089 | 1.00 | 0.00 H |
| ATOM | 111 1HE | MET A | 10133.578 | 7.985 | -7.834 | 1.00 | 0.00 H |
| ATOM | 112 2HE | MET A | 10131.954 | 7.464 | -8.281 | 1.00 | 0.00 H |
| ATOM | 113 3HE | MET A | 10133.312 | 6.350 | -8.437 | 1.00 | 0.00 H |
| ATOM | 114 N | PRO A | 11132.008 | 11.991 | -3.245 | 1.00 | 0.00 N |
| ATOM | 115 CA | PRO A | 11132.361 | 13.332 | -3.719 | 1.00 | 0.00 C |
| ATOM | 116 C | PRO A | 11133.857 | 13.483 | -3.993 | 1.00 | 0.00 C |
| ATOM | 117 O | PRO A | 11134.251 | 14.000 | -5.038 | 1.00 | 0.00 O |
| ATOM | 118 CB | PRO A | 11131.929 | 14.253 | -2.573 | 1.00 | 0.00 C |
| ATOM | 119 CG | PRO A | 11130.928 | 13.466 | -1.798 | 1.00 | 0.00 C |
| ATOM | 120 CD | PRO A | 11131.334 | 12.027 | -1.935 | 1.00 | 0.00 C |
| ATOM | 121 HA | PRO A | 11131.811 | 13.588 | -4.613 | 1.00 | 0.00 H |
| ATOM | 122 1HB | PRO A | 11132.788 | 14.507 | -1.969 | 1.00 | 0.00 H |
| ATOM | 123 2HB | PRO A | 11131.492 | 15.154 | -2.979 | 1.00 | 0.00 H |
| ATOM | 124 1HG | PRO A | 11130.950 | 13.764 | -0.761 | 1.00 | 0.00 H |
| ATOM | 125 2HG | PRO A | 11129.942 | 13.618 | -2.212 | 1.00 | 0.00 H |
| ATOM | 126 1HD | PRO A | 11132.014 | 11.749 | -1.144 | 1.00 | 0.00 H |
| ATOM | 127 2HD | PRO A | 11130.465 | 11.386 | -1.931 | 1.00 | 0.00 H |
| ATOM | 128 N | PRO A | 12134.718 | 13.035 | -3.058 | 1.00 | 0.00 N |
| ATOM | 129 CA | PRO A | 12136.168 | 13.131 | -3.217 | 1.00 | 0.00 C |

| ATOM | 130 | C | PRO A | 12136.731 | 12.015 | -4.090 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|---------|------|--------|
| ATOM | 131 | О | PRO A | 12137.651 | 12.234 | -4.879 | 1.00 | 0.00 O |
| ATOM | 132 | СВ | PRO A | 12136.677 | 12.999 | - 1.785 | 1.00 | 0.00 C |
| ATOM | 133 | CG | PRO A | 12135.676 | 12.124 | -1.112 | 1.00 | 0.00 C |
| ATOM | 134 | CD | PRO A | 12134.349 | 12.402 | -1.774 | 1.00 | 0.00 C |
| ATOM | 135 | НА | PRO A | 12136.461 | 14.089 | -3.621 | 1.00 | 0.00 H |
| ATOM | 136 | IHB | PRO A | 12137.659 | 12.549 | -1.788 | 1.00 | 0.00 H |
| ATOM | 137 2 | 2HB | PRO A | 12136.720 | 13.974 | -1.323 | 1.00 | 0.00 H |
| ATOM | 138 | IHG | PRO A | 12135.949 | 11.087 | -1.246 | 1.00 | 0.00 H |
| ATOM | 139 2 | 2HG | PRO A | 12135.627 | 12.365 | -0.061 | 1.00 | 0.00 H |
| ATOM | 140 | IHD | PRO A | 12133.815 | 11.479 | -1.940 | 1.00 | 0.00 H |
| ATOM | 141 2 | 2HD | PRO A | 12133.761 | 13.074 | -1.167 | 1.00 | 0.00 H |
| ATOM | 142 | N | GLY A | 13136.173 | 10.818 | -3.944 | 1.00 | 0.00 N |
| ATOM | 143 | CA | GLY A | 13136.632 | 9.684 | -4.726 | 1.00 | 0.00 C |
| ATOM | 144 | С | GLY A | 13136.975 | 8.487 | -3.862 | 1.00 | 0.00 C |
| ATOM | 145 | O | GLY A | 13137.982 | 7.818 | -4.091 | 1.00 | 0.00 O |
| ATOM | 146 | Н | GLY A | 13135.443 | 10.703 | -3.300 | 1.00 | 0.00 H |
| ATOM | 147 | ΙHΑ | GLY A | 13135.855 | 9.402 | -5.421 | 1.00 | 0.00 H |
| ATOM | 148 2 | 2HA | GLY A | 13137.510 | 9.976 | -5.283 | 1.00 | 0.00 H |
| ATOM | 149 | N | ASN A | 14136.136 | 8.216 | -2.867 | 1.00 | 0.00 N |
| ATOM | 150 | CA | ASN A | 14136.356 | 7.092 | -1.966 | 1.00 | 0.00 C |
| ATOM | 151 | C | ASN A | 14135.123 | 6.196 | -1.901 | 1.00 | 0.00 C |
| ATOM | 152 | O | ASN A | 14133.991 | 6.673 | -1.989 | 1.00 | 0.00 O |
| ATOM | 153 | CB | ASN A | 14136.708 | 7.595 | -0.565 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14138.013 | 8.366 | -0.540 | 1.00 | 0.00 C |
| ATOM | 155 | OD1 | ASN A | 14138.027 | 9.590 | -0.676 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14139.119 | 7.653 | -0.365 | 1.00 | 0.00 N |

| ATOM | 157 | Н | ASN A | 14135.350 | 8.787 | -2.737 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 158 | НА | ASN A | 14137.185 | 6.515 | -2.350 | 1.00 | 0.00 H |
| ATOM | 159 | 1HB | ASN A | 14135.920 | 8.245 | -0.214 | 1.00 | 0.00 H |
| ATOM | 160 | 2HB | ASN A | 14136.797 | 6.751 | 0.102 | 1.00 | 0.00 H |
| ATOM | 161 | 1HD2 | ASN A | 14139.032 | 6.682 | -0.263 | 1.00 | 0.00 H |
| ATOM | 162 | 2HD2 | ASN A | 14139.977 | 8.127 | -0.344 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15135.349 | 4.896 | -1.747 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15134.257 | 3.933 | -1.670 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15133.351 | 4.234 | -0.480 | 1.00 | 0.00 C |
| ATOM | 166 | О | SER A | 15132.125 | 4.183 | -0.592 | 1.00 | 0.00 O |
| ATOM | 167 | CB | SER A | 15134.808 | 2.511 | -1.559 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15133.762 | 1.569 | -1.395 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15136.274 | 4.576 | -1.683 | 1.00 | 0.00 H |
| ATOM | 170 | НА | SER A | 15133.678 | 4.015 | -2.578 | 1.00 | 0.00 H |
| ATOM | 171 | 1HB | SER A | 15135.357 | 2.269 | -2.456 | 1.00 | 0.00 H |
| ATOM | 172 | 2HB | SER A | 15135.469 | 2.450 | -0.705 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15133.843 | 0.882 | -2.061 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16133.961 | 4.548 | 0.657 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.209 | 4.857 | 1.868 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16134.054 | 5.675 | 2.839 | 1.00 | 0.00 C |
| ATOM | 177 | Ο. | HIS A | 16133.627 | 6.726 | 3.317 | 1.00 | 0.00 O |
| ATOM | 178 | CB | HIS A | 16132.738 | 3.568 | 2.544 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16131.347 | 3.167 | 2.163 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16130.235 | 3.926 | 2.465 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16130.889 | 2.079 | 1.500 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16129.154 | 3.321 | 2.004 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16129.523 | 2.200 | 1.414 | 1.00 | 0.00 N |

| ATOM | 184 H | HIS A | 16134.940 | 4.572 | 0.684 | 1.00 | 0.00 H |
|------|---------|----------|-----------|-------|--------|--------|--------|
| ATOM | 185 H. | A HIS A | 16132.346 | 5.439 | 1.582 | 1.00 | 0.00 H |
| ATOM | 186 1HE | B HIS A | 16133.402 | 2.762 | 2.269 | 1.00 | 0.00 H |
| ATOM | 187 2HE | B HIS A | 16132.765 | 3.700 | 3.616 | 1.00 | 0.00 H |
| ATOM | 188 H | D1 HIS A | 16130.238 | 4.780 | 2.945 | 1.00 | 0.00 H |
| ATOM | 189 H | D2 HIS A | 16131.487 | 1.267 | 1.110 | 1.00 | 0.00 H |
| ATOM | 190 H | E1 HIS A | 16128.141 | 3.684 | 2.094 | 1.00 | 0.00 H |
| ATOM | 191 H | E2 HIS A | 16128.912 | 1.519 | 1.063 | 1.00 | 0.00 H |
| ATOM | 192 N | GLY A | 17135.256 | 5.187 | 3.127 | 1.00 | 0.00 N |
| ATOM | 193 C | A GLY A | 17136.143 | 5.884 | 4.039 | 1.00 | 0.00 C |
| ATOM | 194 C | GLY A | 17137.538 | 5.294 | 4.059 | 1.00 | 0.00 C |
| ATOM | 195 O | GLY A | 17138.056 | 4.942 | 5.119 | 1.00 | 0.00 O |
| ATOM | 196 H | GLY A | 17135.544 | 4.345 | 2.716 | 1.00 | 0.00 H |
| ATOM | 197 1HA | GLY A | 17136.206 | 6.921 | 3.740 | 1.00 | 0.00 H |
| ATOM | 198 2HA | GLY A | 17135.728 | 5.835 | 5.036 | 1.00 | 0.00 H |
| ATOM | 199 N | LEU A | 18138.149 | 5.184 | 2.883 | 1.00 | 0.00 N |
| ATOM | 200 CA | A LEUA | 18139.492 | 4.631 | 2.770 | 1.00 | 0.00 C |
| ATOM | 201 C | LEU A | 18140.541 | 5.657 | 3.188 | 1.00 | 0.00 C |
| ATOM | 202 O | LEU A | 18140.936 | 6.512 | 2.396 | ` 1.00 | 0.00 O |
| ATOM | 203 CI | B LEUA | 18139.758 | 4.170 | 1.335 | 1.00 | 0.00 C |
| ATOM | 204 C | G LEUA | 18138.859 | 3.033 | 0.845 | 1.00 | 0.00 C |
| ATOM | 205 CI | O1 LEU A | 18138.767 | 3.043 | -0.673 | 1.00 | 0.00 C |
| ATOM | 206 CI | D2 LEU A | 18139.378 | 1.691 | 1.341 | 1.00 | 0.00 C |
| ATOM | 207 H | LEU A | 18137.684 | 5.482 | 2.074 | 1.00 | 0.00 H |
| ATOM | 208 H | A LEUA | 18139.558 | 3.778 | 3.429 | 1.00 | 0.00 H |
| ATOM | 209 1HE | B LEUA | 18139.624 | 5.016 | 0.677 | 1.00 | 0.00 H |
| ATOM | 210 2HE | B LEUA | 18140.784 | 3.841 | 1.268 | 1.00 | 0.00 H |

| ATOM | 211 | HG | LEU A | 18137.863 | 3.174 | 1.239 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|-------|--------|------|---------------------|
| ATOM | 212 | 1HD1 | LEU A | 18139.705 | 3.382 | -1.088 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18137.975 | 3.707 | -0.982 | 1.00 | 0.00 H |
| ATOM | 214 | 3HD1 | LEU A | 18138.559 | 2.043 | -1.028 | 1.00 | 0.00 H |
| ATOM | 215 | 1HD2 | LEU A | 18139.928 | 1.837 | 2.260 | 1.00 | 0.00 H |
| ATOM | 216 | 2HD2 | LEU A | 18140.029 | 1.260 | 0.596 | 1.00 | 0.00 H |
| ATOM | 217 | 3HD2 | LEU A | 18138.546 | 1.028 | 1.521 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19140.986 | 5.564 | 4.436 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.989 | 6.485 | 4.959 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19143.037 | 5.739 | 5.779 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19142.979 | 4.517 | 5.913 | 1.00 | 0.00 O |
| ATOM | 222 | СВ | GLU A | 19141.325 | 7.562 | 5.819 | 1.00 | 0.00 _, C |
| ATOM | 223 | CG | GLU A | 19140.463 | 7.001 | 6.937 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19139.402 | 7.979 | 7.402 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19139.434 | 8.369 | 8.589 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19138.541 | 8.356 | 6.581 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.633 | 4.861 | 5.019 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.476 | 6.957 | 4.119 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19142.094 | 8.179 | 6.260 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19140.701 | 8.176 | 5.186 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.974 | 6.106 | 6.584 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19141.098 | 6.756 | 7.776 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.994 | 6.483 | 6.324 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL A | 20145.055 | 5.891 | 7.131 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.481 | 5.136 | 8.326 | 1.00 | 0.00 C |
| ATOM | 236 | О | VAL A | 20143.631 | 5.653 | 9.050 | 1.00 | 0.00 O |
| ATOM | 237 | СВ | VALA | 20146.037 | 6.964 | 7.639 | 1.00 | 0.00 C |

| ATOM | 238 | CG1 | VAL A | 20147.209 | 6.320 | 8.365 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 239 | CG2 | VALA | 20146.525 | 7.828 | 6.485 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VALA | 20143.987 | 7.452 | 6.181 | 1.00 | 0.00 H |
| ATOM | 241 | HA | VAL A | 20145.601 | 5.198 | 6.508 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.515 | 7.600 | 8.339 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VALA | 20148.077 | 6.958 | 8.284 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20147.425 | 5.361 | 7.919 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20146.957 | 6.185 | 9.406 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20145.737 | 8.499 | 6.179 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20146.802 | 7.196 | 5.655 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20147.384 | 8.402 | 6.803 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.950 | 3.908 | 8.525 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.472 | 3.102 | 9.631 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.364 | 2.152 | 9.221 | 1.00 | 0.00 C |
| ATOM | 252 | О | GLY A | 21143.223 | 1.069 | 9.789 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.627 | 3.547 | 7.913 | 1.00 | 0.00 H |
| ATOM | 254 | 1HA | GLY A | 21145.296 | 2.526 | 10.025 | 1.00 | 0.00 H |
| ATOM | 255 | 2HA | GLY A | 21144.102 | 3.757 | 10.406 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.573 | 2.559 | 8.232 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.471 | 1.736 | 7.747 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.972 | 0.673 | 6.775 | 1.00 | 0.00 C |
| ATOM | 259 | О | SER A | 22142.811 | 0.948 | 5.916 | 1.00 | 0.00 O |
| ATOM | 260 | CB | SER A | 22140.417 | 2.611 | 7.066 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22139.648 | 3.320 | 8.022 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.735 | 3.432 | 7.820 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22141.024 | 1.246 | 8.598 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.907 | 3.322 | 6.417 | 1.00 | 0.00 H |

| ATOM | 265 | 2HB | SER A | 22139.756 | 1.986 | 6.482 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 266 | HG | SER A | 22140.233 | 3.756 | 8.644 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.454 | -0.542 | 6.915 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.848 | -1.647 | 6.049 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.271 | -1.474 | 4.649 | 1.00 | 0.00 C |
| ATOM | 270 | Ο | LEU A | 23140.212 | -0.873 | 4.474 | 1.00 | 0.00 O |
| ATOM | 271 | СВ | LEU A | 23141.386 | -2.979 | 6.644 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23142.034 | -3.354 | 7.977 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23141.095 | -4.216 | 8.805 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.354 | -4.074 | 7.743 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.789 | -0.700 | 7.620 | 1.00 | 0.00 H |
| ATOM | 276 | НА | LEU A | 23142.926 | -1.648 | 5.984 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.316 | -2.931 | 6.788 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.602 | -3.761 | 5.932 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.239 | -2.452 | 8.537 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23140.088 | -3.834 | 8.720 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23141.402 | -4.193 | 9.840 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23141.125 | -5.232 | 8.442 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23143.989 | -3.950 | 8.607 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23143.843 | -3.657 | 6.874 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23143.167 | -5.125 | 7.581 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24141.975 | -2.007 | 3.654 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.532 | -1.911 | 2.269 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.129 | -3.030 | 1.423 | 1.00 | 0.00 C |
| ATOM | 289 | О | ALA A | 24142.995 | -3.774 | 1.883 | 1.00 | 0.00 O |
| ATOM | 290 | CB | ALA A | 24141.902 | -0.554 | 1.689 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.811 | -2.474 | 3.858 | 1.00 | 0.00 H |

| ATOM | 292 | HA | ALA A | 24140.455 | -1.999 | 2.256 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 293 1 | HB | ALA A | 24142.966 | -0.395 | 1.797 | 1.00 | 0.00 H |
| ATOM | 294 2 | 2HB | ALA A | 24141.367 | 0.221 | 2.216 | 1.00 | 0.00 H |
| ATOM | 295 3 | ВНВ | ALA A | 24141.638 | -0.525 | 0.642 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.660 | -3.144 | 0.185 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.147 | -4.174 | -0.726 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.482 | -3.580 | -2.090 | 1.00 | 0.00 C |
| ATOM | 299 | O | GLU A | 25141.969 | -2.524 | -2.461 | 1.00 | 0.00 O |
| ATOM | 300 | СВ | GLU A | 25141.105 | -5.282 | -0.880 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.622 | -6.505 | -1.622 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.539 | -7.537 | -1.869 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25139.448 | -7.152 | -2.336 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25140.785 | -8.732 | -1.597 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25140.969 | -2.522 | -0.124 | 1.00 | 0.00 H |
| ATOM | 306 | HA | GLU A | 25143.047 | -4.594 | -0.299 | 1.00 | 0.00 H |
| ATOM | 307 1 | HB | GLU A | 25140.778 | -5.594 | 0.100 | 1.00 | 0.00 H |
| ATOM | 308 2 | ΣHB | GLU A | 25140.258 | -4.890 | -1.424 | 1.00 | 0.00 H |
| ATOM | 309 1 | HG | GLU A | 25142.022 | -6.190 | -2.575 | 1.00 | 0.00 H |
| ATOM | 310 2 | 2HG | GLU A | 25142.407 | -6.960 | -1.035 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.346 | -4.266 | -2.833 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.749 | -3.806 | -4.157 | 1.00 | 0.00 C |
| ATOM | 313 | C | VALA | 26143.397 | -4.834 | -5.227 | 1.00 | 0.00 C |
| ATOM | 314 | O | VAL A | 26143.403 | -6.038 | -4.971 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VAL A | 26145.261 | -3.520 | -4.216 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VAL A | 26145.630 | -2.857 | -5.534 | 1.00 | 0.00 C |
| ATOM | 317 | CG2 | VAL A | 26145.688 | -2.657 | -3.038 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.721 | -5.100 | -2.482 | 1.00 | 0.00 H |

| ATOM | 319 | HA | VAL A | 26143.221 | -2.886 | -4.366 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|---------|------|--------|
| ATOM | 320 | НВ | VAL A | 26145.788 | -4.461 | -4.153 | 1.00 | 0.00 H |
| ATOM | 321 | 1HG1 | VAL A | 26144.767 | -2.343 | -5.931 | 1.00 | 0.00 H |
| ATOM | 322 | 2HG1 | VAL A | 26145.957 | -3.609 | -6.236 | 1.00 | 0.00 H |
| ATOM | 323 | 3HG1 | VAL A | 26146.427 | -2.146 | -5.370 | 1.00 | 0.00 H |
| ATOM | 324 | 1HG2 | VALA | 26145.118 | -1.739 | -3.039 | 1.00 | 0.00 H |
| ATOM | 325 | 2HG2 | VAL A | 26146.740 | -2.427 | -3.122 | 1.00 | 0.00 H |
| ATOM | 326 | 3HG2 | VAL A | 26145.508 | -3.190 | -2.117 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYS A | 27143.090 | -4.350 | -6.425 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27142.735 | -5.226 | -7.536 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27143.971 | -5.609 | -8.343 | 1.00 | 0.00 C |
| ATOM | 330 | О | LYS A | 27144.276 | -4.991 | -9.362 | 1.00 | 0.00 O |
| ATOM | 331 | CB | LYS A | 27141.708 | -4.544 | -8.443 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.274 | -4.963 | -8.160 | 1.00 | 0.00 C |
| ATOM | 33,3 | CD | LYS A | 27139.289 | -4.199 | -9.032 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27138.175 | -5.101 | -9.536 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27138.653 | -6.038 | -10.591 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27143.103 | -3.380 | -6.567 | 1.00 | 0.00 H |
| ATOM | 337 | HA | LYS A | 27142.297 | -6.123 | -7.123 | 1.00 | 0.00 H |
| ATOM | 338 | 1HB | LYS A | 27141.781 | -3.475 | -8.309 | 1.00 | 0.00 H |
| ATOM | 339 | 2HB | LYS A | 27141.934 | -4.786 | -9.470 | 1.00 | 0.00 H |
| ATOM | 340 | 1HG | LYS A | 27140.171 | -6.019 | -8.360 | 1.00 | 0.00 H |
| ATOM | 341 | 2HG | LYS A | 27140.050 | -4.766 | -7.122 | 1.00 | 0.00 H |
| ATOM | 342 | 1HD | LYS A | 27138.855 | -3.399 | -8.451 | 1.00 | 0.00 H |
| ATOM | 343 | 2HD | LYS A | 27139.818 | -3.785 | -9.879 | 1.00 | 0.00 H |
| ATOM | 344 | 1HE | LYS A | 27137.790 | -5.675 | -8.707 | 1.00 | 0.00 H |
| ATOM | 345 | 2HE | LYS A | 27137.388 | -4.486 | -9.945 | 1.00 | 0.00 H |

ATOM 346 1HZ LYS A 27139.312 -5.550 -11.231 0.00 H 1.00 **ATOM** 347 2HZ LYS A 27137.849 -6.394 -11.145 1.00 0.00 H348 3HZ LYS A 27139.145 -6.845 -10.156 1.00 **ATOM** 0.00 HGLU A 28144.679 -6.635 -7.880 1.00 0.00 N **ATOM** 349 N **ATOM** 350 CA GLUA 28145.883 -7.101 -8.559 1.00 0.00 C C GLUA 28145.850 -8.615 -8.743 1.00 0.00 C **ATOM** 351 Ο GLUA 28144.881 -9.276 -8.371 1.00 0.00 O **ATOM** 352 **ATOM** 353 CB GLUA 28147.129 -6.694 -7.770 1.00 0.00 C **ATOM** CG GLUA 28148.209 -6.054 -8.627 1.00 0.00 C 354 CD GLUA 28147.852 -4.643 -9.054 1.00 0.00 C **ATOM** 355 **ATOM** 356 OE1 GLU A 28147.828 -4.382 -10.276 1.00 0.00 O OE2 GLU A 28147.598 -3.801 -8.168 1.00 0.00 O **ATOM** 357 GLUA 28144.386 -7.089 -7.063 1.00 0.00 H **ATOM** 358 Η -9.532 359 HA GLUA 28145.915 -6.634 1.00 0.00 H **ATOM ATOM** 360 1HB GLU A 28146.842 -5.989 -7.005 1.00 0.00 H **ATOM** 361 2HB GLU A 28147.548 -7.573 -7.299 1.00 0.00 H **ATOM** 362 1HG GLUA 28149.127 -6.021 -8.060 1.00 0.00 H -9.511 363 2HG GLUA 28148.355 -6.657 1.00 0.00 H **ATOM ATOM** 364 N ASN A 29146.918 -9.159 -9.319 1.00 0.00 N 365 CA ASNA 29147.013 -10.595 -9.551 1.00 0.00 C **ATOM ATOM** 366 -C ASN A 29147.022 -11.360 -8.230 1.00 0.00 C **ATOM** 367 O ASN A 29146.158 -12.203 -7.987 1.00 0.00 O **ATOM** CBASN A 29148.275 -10.920 -10.354 1.00 0.00 C 368 369 CG ASNA 29147.996 -11.056 -11.838 1.00 0.00 C **ATOM** OD1 ASN A 29147.912 -12.164 -12.367 1.00 0.00 O **ATOM** 370 ND2 ASN A 29147.853 -9.925 -12.519 1.00 0.00 N **ATOM** 371 **ATOM** 372 H ASN A 29147.660 -8.580 -9.594 1.00 0.00 H

| ATOM | 373 | НА | ASN A | 29146.146 | -10.896 | -10.121 | 1.00 | 0.00 H |
|------|--------------|------|-------|-----------|-----------|---------|------|--------|
| ATOM | 374 | 1HB | ASN A | 29148.997 | -10.130 - | 10.214 | 1.00 | 0.00 H |
| ATOM | 375 2 | 2HB | ASN A | 29148.691 | -11.852 | -9.998 | 1.00 | 0.00 H |
| ATOM | 376 | HD2 | ASN A | 29147.934 | -9.078 - | 12.031 | 1.00 | 0.00 H |
| ATOM | 377 2 | 2HD2 | ASN A | 29147.672 | -9.983 - | 13.480 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30148.002 | -11.075 | -7.356 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30148.120 | -11.741 | -6.056 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30147.114 | -11.205 | -5.038 | 1.00 | 0.00 C |
| ATOM | 381 | O | PRO A | 30147.237 | -10.072 | -4.573 | 1.00 | 0.00 O |
| ATOM | 382 | СВ | PRO A | 30149.546 | -11.404 | -5.625 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30149.829 | -10.088 | -6.263 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30149.076 | -10.083 | -7.567 | 1.00 | 0.00 C |
| ATOM | 385 | HA | PRO A | 30148.011 | -12.810 | -6.147 | 1.00 | 0.00 H |
| ATOM | 386 | lНВ | PRO A | 30149.593 | -11.340 | -4.546 | 1.00 | 0.00 H |
| ATOM | 387 2 | 2HB | PRO A | 30150.223 | -12.167 | -5.977 | 1.00 | 0.00 H |
| ATOM | 388 | IHG | PRO A | 30149.481 | -9.289 | -5.626 | 1.00 | 0.00 H |
| ATOM | 389 2 | 2HG | PRO A | 30150.890 | -9.989 | -6.444 | 1.00 | 0.00 H |
| ATOM | 390 1 | IHD | PRO A | 30148.662 | -9.105 | -7.757 | 1.00 | 0.00 H |
| ATOM | 391 2 | 2HD | PRO A | 30149.722 | -10.382 | -8.377 | 1.00 | 0.00 H |
| ATOM | 392 | N | PRO A | 31146.100 | -12.014 | -4.676 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31145.077 | -11.606 | -3.707 | 1.00 | 0.00 C |
| ATOM | 394 | C | PRO A | 31145.637 | -11.476 | -2.293 | 1.00 | 0.00 C |
| ATOM | 395 | O | PRO A | 31145.647 | -12.440 | -1.529 | 1.00 | 0.00 O |
| ATOM | 396 | CB | PRO A | 31144.050 | -12.738 | -3.773 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31144.818 | -13.920 | -4.250 | 1.00 | 0.00 C |
| ATOM | 398 | CD | PRO A | 31145.872 | -13.382 | -5.177 | 1.00 | 0.00 C |
| ATOM | 399 | HA | PRO A | 31144.611 | -10.675 | -3.994 | 1.00 | 0.00 H |

| ATOM | 400 1 | НВ | PRO A | 31143.633 | -12.906 | -2.791 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|-----------------|------|--------|
| ATOM | 401 2 | 2HB | PRO A | 31143.263 | -12.474 | -4.464 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31145.278 | -14.423 | -3.411 > | 1.00 | 0.00 H |
| ATOM | 403 2 | 2HG | PRO A | 31144.163 | -14.596 | -4.779 | 1.00 | 0.00 H |
| ATOM | 404 1 | HD | PRO A | 31146.773 | -13.973 | -5.109 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31145.507 | -13.363 | -6.193 | 1.00 | 0.00 H |
| ATOM | 406 | N | PHE A | 32146.101 | -10.278 | -1.955 | 1.00 | 0.00 N |
| ATOM | 407 | CA | PHE A | 32146.662 | -10.020 | -0.634 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.773 | -9.069 | 0.160 | 1.00 | 0.00 C |
| ATOM | 409 | O | PHE A | 32144.803 | -8.524 | -0.368 | 1.00 | 0.00 O |
| ATOM | 410 | CB | PHE A | 32148.070 | -9.434 | -0.760 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.162 | -8.301 | -1.742 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.899 | -8.435 | -2.907 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32147.511 | -7.102 | -1.499 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.985 | -7.394 | -3.813 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.593 | -6.057 | -2.400 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.331 | -6.203 | -3.558 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32146.065 | -9.548 | -2.609 | 1.00 | 0.00 H |
| ATOM | 418 | HA | PHE A | 32146.721 | -10.962 | -0.109 | 1.00 | 0.00 H |
| ATOM | 419 1 | HB | PHE A | 32148.386 | -9.064 | 0.204 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.748 | -10.211 | -1.083 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32149.409 | -9.365 | -3.107 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32146.933 | -6.987 | -0.593 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32149.563 | -7.510 | -4.717 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32147.082 | -5.128 | -2.199 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.397 | -5.389 | -4.264 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.109 | -8.875 | 1.431 | 1.00 | 0.00 N |

| ATOM | 427 | CA | TYR A | 33145.340 | -7.989 | 2.298 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 428 | С | TYR A | 33146.263 | -7.088 | 3.112 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.282 | -7.538 | 3.635 | 1.00 | 0.00 O |
| ATOM | 430 | СВ | TYR A | 33144.448 | -8.807 | 3.236 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.132 | -9.218 | 2.616 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.336 | -8.293 | 1.954 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.687 - | 10.531 | 2.692 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.131 | -8.664 | 1.386 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.485 | 10.911 | 2.126 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.711 | -9.974 | 1.474 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.514 | -10.348 | 0.910 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.892 | -9.337 | 1.795 | 1.00 | 0.00 H |
| ATOM | 439 | НА | TYR A | 33144.715 | -7.371 | 1.670 | 1.00 | 0.00 H |
| ATOM | 440 | НВ | TYR A | 33144.972 | -9.705 | 3.527 | 1.00 | 0.00 H |
| ATOM | 441 2 | 2HB | TYR A | 33144.233 | -8.221 | 4.117 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33142.667 | -7.267 | 1.885 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33143.295 | -11.264 | 3.203 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33140.527 | -7.930 | 0.875 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33141.156 - | 11.937 | 2.196 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.057 | -10.955 | 1.498 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.899 | -5.814 | 3.214 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.705 | -4.871 | 3.966 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34145.905 | -3.675 | 4.442 | 1.00 | 0.00 C |
| ATOM | 450 | O | GLY A | 34144.740 | -3.513 | 4.077 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.075 | -5.513 | 2.776 | 1.00 | 0.00 H |
| ATOM | 452 | lΗA | GLY A | 34147.123 | -5.375 | 4.825 | 1.00 | 0.00 H |
| ATOM | 453 2 | 2HA | GLY A | 34147.511 | -4.524 | 3.338 | 1.00 | 0.00 H |

| ATOM | 454 | N | VAL A | 35146.531 | -2.835 | 5.261 | 1.00 | 0.00 N |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 455 | CA | VAL A | 35145.870 | -1.647 | 5.789 | 1.00 | 0.00 C |
| ATOM | 456 | C | VAL A | 35146.552 | -0:375 | 5.292 | 1.00 | 0.00 C |
| ATOM | 457 | Ο | VAL A | 35147.766 | -0.345 | 5.095 | 1.00 | 0.00 O |
| ATOM | 458 | CB | VAL A | 35145.861 | -1.649 | 7.330 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.281 | -1.641 | 7.878 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35145.069 | -0.464 | 7.864 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.459 | -3.018 | 5.515 | 1.00 | 0.00 H |
| ATOM | 462 | НА | VAL A | 35144.846 | -1.653 | 5.443 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.378 | -2.556 | 7.665 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VAL A | 35147.861 | -0.890 | 7.361 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35147.730 | -2.611 | 7.726 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VAL A | 35147.259 | -1.415 | 8.934 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VAL A | 35144.397 | -0.107 | 7.098 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VAL A | 35145.749 | 0.326 | 8.144 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VAL A | 35144.500 | -0.772 | 8.729 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.761 | 0.675 | 5.093 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.289 | 1.949 | 4.620 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.261 | 2.548 | 5.632 | 1.00 | 0.00 C |
| ATOM | 473 | О | ILE A | 36147.108 | 2.361 | 6.840 | 1.00 | 0.00 O |
| ATOM | 474 | СВ | ILE A | 36145.160 | 2.962 | 4.345 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.100 | 2.342 | 3.431 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILE A | 36145.726 | 4.232 | 3.724 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.962 | 3.283 | 3.101 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.801 | 0.591 | 5.268 | 1.00 | 0.00 H |
| ATOM | 479 | НА | ILE A | 36146.816 | 1.768 | 3.695 | 1.00 | 0.00 H |
| ATOM | 480 | НВ | ILE A | 36144.704 | 3.224 | 5.288 | 1.00 | 0.00 H |

| ATOM | 481 1HG1 | ILEA 3 | 36144.564 | 2.046 | 2.502 | 1.00 | 0.00 H |
|------|----------|--------|-----------|-------|--------|------|--------|
| ATOM | 482 2HG1 | ILE A | 36143.683 | 1.472 | 3.913 | 1.00 | 0.00 H |
| ATOM | 483 1HG2 | ILE A | 36146.440 | 4.677 | 4.402 | 1.00 | 0.00 H |
| ATOM | 484 2HG2 | ILE A | 36144.923 | 4.930 | 3.538 | 1.00 | 0.00 H |
| ATOM | 485 3HG2 | ILE A | 36146.216 | 3.989 | 2.794 | 1.00 | 0.00 H |
| ATOM | 486 1HD1 | ILE A | 36143.360 | 4.209 | 2.712 | 1.00 | 0.00 H |
| ATOM | 487 2HD1 | ILE A | 36142.390 | 3.485 | 3.995 | 1.00 | H 00.0 |
| ATOM | 488 3HD1 | ILE A | 36142.321 | 2.827 | 2.360 | 1.00 | 0.00 H |
| ATOM | 489 N | ARG A | 37148.260 | 3.266 | 5.132 | 1.00 | 0.00 N |
| ATOM | 490 CA | ARG A | 37149.257 | 3.890 | 5.993 | 1.00 | 0.00 C |
| ATOM | 491 C | ARG A | 37149.449 | 5.360 | 5.629 | 1.00 | 0.00 C |
| ATOM | 492 O | ARG A | 37149.125 | 6.251 | 6.413 | 1.00 | 0.00 O |
| ATOM | 493 CB | ARG A | 37150.590 | 3.149 | 5.885 | 1.00 | 0.00 C |
| ATOM | 494 CG | ARG A | 37150.463 | 1.645 | 6.063 | 1.00 | 0.00 C |
| ATOM | 495 CD | ARG A | 37150.492 | 1.254 | 7.532 | 1.00 | 0.00 C |
| ATOM | 496 NE | ARG A | 37149.280 | 1.671 | 8.234 | 1.00 | 0.00 N |
| ATOM | 497 CZ | ARG A | 37149.190 | 1.779 | 9.558 | 1.00 | 0.00 C |
| ATOM | 498 NH1 | ARG A | 37150.236 | 1.502 | 10.326 | 1.00 | 0.00 N |
| ATOM | 499 NH2 | ARG A | 37148.049 | 2.166 | 10.114 | 1.00 | 0.00 N |
| ATOM | 500 H | ARG A | 37148.330 | 3.378 | 4.161 | 1.00 | 0.00 H |
| ATOM | 501 HA | ARG A | 37148.903 | 3.828 | 7.011 | 1.00 | 0.00 H |
| ATOM | 502 1HB | ARG A | 37151.018 | 3.340 | 4.912 | 1.00 | 0.00 H |
| ATOM | 503 2HB | ARG A | 37151.261 | 3.524 | 6.644 | 1.00 | 0.00 H |
| ATOM | 504 1HG | ARG A | 37149.529 | 1.318 | 5.633 | 1.00 | 0.00 H |
| ATOM | 505 2HG | ARG A | 37151.286 | 1.161 | 5.556 | 1.00 | 0.00 H |
| ATOM | 506 1HD | ARG A | 37150.587 | 0.181 | 7.604 | 1.00 | 0.00 H |
| ATOM | 507 2HD | ARG A | 37151.345 | 1.722 | 7.999 | 1.00 | 0.00 H |

| ATOM | 508 | HE | ARG A | 37148.493 | 1.881 | 7.691 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 509 | 1HH1 | ARG A | 37151.098 | 1.209 | 9.913 | 1.00 | 0.00 H |
| ATOM | 510 | 2HH1 | ARG A | 37150.161 | 1.585 | 11.320 | 1.00 | 0.00 H |
| ATOM | 511 | 1HH2 | ARG A | 37147.259 | 2.376 | 9.540 | 1.00 | 0.00 H |
| ATOM | 512 | 2HH2 | ARG A | 37147.982 | 2.247 | 11.108 | 1.00 | 0.00 H |
| ATOM | 513 | N | TRPA | 38149.977 | 5.605 | 4.434 | 1.00 | 0.00 N |
| ATOM | 514 | CA | TRPA | 38150.210 | 6.967 | 3.968 | 1.00 | 0.00 C |
| ATOM | 515 | C | TRPA | 38149.461 | 7.233 | 2.665 | 1.00 | 0.00 C |
| ATOM | 516 | O | TRPA | 38149.556 | 6.459 | 1.712 | 1.00 | 0.00 O |
| ATOM | 517 | CB | TRPA | 38151.709 | 7.216 | 3.772 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38152.013 | 8.486 | 3.032 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRP A | 38152.250 | 9.716 | 3.576 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRP A | 38152.100 | 8.650 | 1.612 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRPA | 38152.480 | 10.635 | 2.580 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.395 | 10.004 | 1.365 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38151.959 | 7.782 | 0.525 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRPA | 38152.550 | 10.509 | 0.076 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.114 | 8.285 | -0.753 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRPA | 38152.406 | 9.637 | -0.968 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRPA | 38150.215 | 4.852 | 3.852 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRPA | 38149.839 | 7.642 | 4.724 | 1.00 | 0.00 H |
| ATOM | 529 | 1HB | TRPA | 38152.188 | 7.272 | 4.739 | 1.00 | 0.00 H |
| ATOM | 530 | 2HB | TRPA | 38152.134 | 6.395 | 3.212 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38152.253 | 9.922 | 4.636 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38152.676 | 11.585 | 2.716 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRP A | 38151.734 | 6.737 | 0.672 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRP A | 38152.772 | 11.549 | -0.107 | 1.00 | 0.00 H |

| ATOM | 535 | HZ3 | TRP A | 38152.009 | 7.629 | -1.604 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 536 | HH2 | TRP A | 38152.519 | 9.986 | -1.984 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.726 | 8.338 | 2.631 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39147.967 | 8.719 | 1.446 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILĖ A | 39148.411 | 10.088 | 0.940 | 1.00 | 0.00 C |
| ATOM | 540 | O | ILE A | 39148.093 | 11.113 | 1.541 | 1.00 | 0.00 O |
| ATOM | 541 | СВ | ILE A | 39146.454 | 8.753 | 1.731 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39146.012 | 7.460 | 2.417 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.675 | 8.969 | 0.442 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.676 | 7.574 | 3.117 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.697 | 8.917 | 3.421 | 1.00 | 0.00 H |
| ATOM | 546 | НА | ILE A | 39148.154 | 7.983 | 0.677 | 1.00 | 0.00 H |
| ATOM | 547 | HB | ILE A | 39146.253 | 9.587 | 2.386 | 1.00 | 0.00 H |
| ATOM | 548 | 1HG1 | ILE A | 39145.933 | 6.677 | 1.678 | 1.00 | 0.00 H |
| ATOM | 549 | 2HG1 | ILE A | 39146.751 | 7.181 | 3.154 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39144.625 | 8.799 | 0.623 | 1.00 | 0.00 H |
| ATOM | 551 | 2HG2 | ILE A | 39146.028 | 8.278 | -0.310 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39145.822 | 9.982 | 0.098 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.179 | 8.477 | 2.800 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39144.830 | 7.604 | 4.186 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39144.064 | 6.719 | 2.866 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.152 | 10.097 | -0.164 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.630 | 11.349 | -0.720 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.140 | 11.202 | -2.140 | 1.00 | 0.00 C |
| ATOM | 559 | Ο | GLY A | 40149.996 | 10.144 | -2.755 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.379 | 9.250 | -0.599 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40148.823 | 12.064 | -0.713 | 1.00 | 0.00 H |

| ATOM | 562 | 2HA | GLY A | 40150.431 | 11.721 | -0.100 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 563 | N | GLN A | 41150.738 | 12.268 | -2.659 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.275 | 12.266 | -4.014 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41152.744 | 12.682 | -4.013 | 1.00 | 0.00 C |
| ATOM | 566 | О | GLN A | 41153.073 | 13.816 | -3.661 | 1.00 | 0.00 O |
| ATOM | 567 | СВ | GLN A | 41150.463 | 13.213 | -4.899 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41148.960 | 13.014 | -4.785 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.199 | 14.324 | -4.770 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.192 | 15.042 | -3.770 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41147.550 | 14.643 | -5.884 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41150.820 | 13.080 | -2.117 | 1.00 | 0.00 H |
| ATOM | 573 | НА | GLN A | 41151.192 | 11.264 | -4.405 | 1.00 | 0.00 H |
| ATOM | 574 | lНВ | GLN A | 41150.692 | 14.230 | -4.618 | 1.00 | 0.00 H |
| ATOM | 575 2 | 2HB | GLN A | 41150.750 | 13.060 | -5.927 | 1.00 | 0.00 H |
| ATOM | 576 | IHG | GLN A | 41148.623 | 12.428 | -5.626 | 1.00 | 0.00 H |
| ATOM | 577 2 | 2HG | GLN A | 41148.750 | 12.481 | -3.869 | 1.00 | 0.00 H |
| ATOM | 578 | HE2 | GLN A | 41147.599 | 14.024 | -6.642 | 1.00 | 0.00 H |
| ATOM | 579 2 | 2HE2 | GLN A | 41147.049 | 15.485 | -5.903 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42153.655 | 11.772 | -4.405 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.092 | 12.061 | -4.440 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.420 | 13.259 | -5.326 | 1.00 | 0.00 C |
| ATOM | 583 | O | PRO A | 42154.629 | 13.637 | -6.191 | 1.00 | 0.00 O |
| ATOM | 584 | CB | PRO A | 42155.706 | 10.783 | -5.022 | 1.00 | 0.00 C |
| ATOM | 585 | CG | PRO A | 42154.698 | 9.719 | -4.754 | 1.00 | 0.00 C |
| ATOM | 586 | CD | PRO A | 42153.361 | 10.395 | -4.841 | 1.00 | 0.00 C |
| ATOM | 587 | НА | PRO A | 42155.484 | 12.233 | -3.448 | 1.00 | 0.00 H |
| ATOM | 588 | 1HB | PRO A | 42155.874 | 10.911 | -6.081 | 1.00 | 0.00 H |

| ATOM | 589 2HB | PRO A | 42156.642 | 10.573 | -4.526 | 1.00 | 0.00 H |
|--------|---------|-------|-----------|----------|--------|------|--------|
| ATOM | 590 1HG | PRO A | 42154.776 | 8.942 | -5.499 | 1.00 | 0.00 H |
| ATOM | 591 2HG | PRO A | 42154.848 | 9.311 | -3.765 | 1.00 | 0.00 H |
| ATOM | 592 1HD | PRO A | 42152.996 | 10.381 | -5.857 | 1.00 | 0.00 H |
| ATOM | 593 2HD | PRO A | 42152.653 | 9.922 | -4.176 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43156.595 | 13.876 | -5.121 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.024 | 15.037 | -5.905 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43157.402 | 14.663 | -7.333 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43158.567 | 14.392 | -7.627 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43158.249 | 15.545 | -5.146 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43158.788 | 14.344 | -4.449 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43157.597 | 13.489 | -4.110 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43156.264 | 15.804 | -5.924 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43158.965 | 15.950 | -5.847 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43157.951 | 16.307 | -4.443 | 1.00 | 0.00 H |
| ATOM | 604 1HG | PRO A | 43159.457 | 13.808 | -5.107 | 1.00 | 0.00 H |
| ATOM | 605 2HG | PRO A | 43159.304 | 14.642 | -3.549 | 1.00 | 0.00 H |
| ATOM | 606 1HD | PRO A | 43157.847 | 12.442 | -4.196 | 1.00 | 0.00 H |
| ATOM | 607 2HD | PRO A | 43157.244 | 13.713 | -3.114 | 1.00 | 0.00 H |
| ATOM | 608 N | GLY A | 44156.412 | 14.650 | -8.219 | 1.00 | 0.00 N |
| ATOM | 609 CA | GLY A | 44156.666 | 14.309 | -9.605 | 1.00 | 0.00 C |
| ATOM | 610 C | GLY A | 44155.424 | 13.817 - | 10.320 | 1.00 | 0.00 C |
| ATOM | 611 O | GLY A | 44155.089 | 14.302 - | 11.401 | 1.00 | 0.00 O |
| ATOM . | 612 H | GLY A | 44155.503 | 14.876 | -7.929 | 1.00 | 0.00 H |
| ATOM | 613 1HA | GLY A | 44157.039 | 15.183 - | 10.117 | 1.00 | 0.00 H |
| ATOM | 614 2HA | GLY A | 44157.418 | 13.535 | -9.641 | 1.00 | 0.00 H |
| ATOM | 615 N | LEU A | 45154.738 | 12.852 | -9.716 | 1.00 | 0.00 N |

| ATOM | 616 | CA | LEU A | 45153.525 | 12.298 | -10.306 | 1.00 | 0.00 C | |
|------|-----|------|---------|-----------|----------|---------|------|--------|--|
| ATOM | 617 | C | LEU A | 45152.337 | 12.469 | -9.368 | 1.00 | 0.00 C | |
| ATOM | 618 | Ο | LEU A | 45152.290 | 11.867 | -8.297 | 1.00 | 0.00 O | |
| ATOM | 619 | CB | LEU A | 45153.722 | 10.815 | -10.630 | 1.00 | 0.00 C | |
| ATOM | 620 | CG | LEU A | 45154.338 | 9.984 | -9.503 | 1.00 | 0.00 C | |
| ATOM | 621 | CD1 | LEU A | 45154.029 | 8.505 | -9.697 | 1.00 | 0.00 C | |
| ATOM | 622 | CD2 | LEUA | 45155.842 | 10.216 | -9.432 | 1.00 | 0.00 C | |
| ATOM | 623 | Н | LEU A | 45155.053 | 12.507 | -8.852 | 1.00 | 0.00 H | |
| ATOM | 624 | HA | LEU A | 45153.326 | 12.833 | -11.222 | 1.00 | 0.00 H | |
| ATOM | 625 | 1HB | LEU A | 45152.760 | 10.391 - | 10.877 | 1.00 | 0.00 H | |
| ATOM | 626 | 2HB | LEU A | 45154.364 | 10.739 - | 11.495 | 1.00 | 0.00 H | |
| ATOM | 627 | HG | LEU A | 45153.907 | 10.292 | -8.561 | 1.00 | 0.00 H | |
| ATOM | 628 | 1HD1 | LEU A | 45153.531 | 8.361 - | 10.644 | 1.00 | 0.00 H | |
| ATOM | 629 | 2HD1 | LEU A | 45153.386 | 8.164 | -8.898 | 1.00 | 0.00 H | |
| ATOM | 630 | 3HD1 | LEU A | 45154.949 | 7.939 | -9.684 | 1.00 | 0.00 H | |
| ATOM | 631 | 1HD2 | LEU A | 45156.072 | 10.818 | -8.566 | 1.00 | 0.00 H | |
| ATOM | 632 | 2HD2 | LEU A | 45156.170 | 10.728 - | 10.324 | 1.00 | 0.00 H | |
| ATOM | 633 | 3HD2 | LEU A | 45156.351 | 9.266 | -9.355 | 1.00 | 0.00 H | |
| ATOM | 634 | N | ASN A | 46151.375 | 13.292 | -9.776 | 1.00 | 0.00 N | |
| ATOM | 635 | CA | ASN A | 46150.192 | 13.528 | -8.962 | 1.00 | 0.00 C | |
| ATOM | 636 | C | ASN A | 46149.268 | 12.316 | -9.000 | 1.00 | 0.00 C | |
| ATOM | 637 | Ο | ASN A | 46148.624 | 12.044 | -10.013 | 1.00 | 0.00 O | |
| ATOM | 638 | CB | ASN A | 46149.446 | 14.769 | -9.454 | 1.00 | 0.00 C | |
| ATOM | 639 | CG | ASN A | 46148.709 | 15.484 | -8.339 | 1.00 | 0.00 C | |
| ATOM | 640 | OD1 | ASN A | 46147.479 | 15.539 | -8.328 | 1.00 | 0.00 O | |
| ATOM | 641 | ND2 | 2 ASN A | 46149.460 | 16.036 | -7.393 | 1.00 | 0.00 N | |
| ATOM | 642 | Н | ASN A | 46151.462 | 13.744 | -10.641 | 1.00 | 0.00 H | |

| ATOM | 643 | HA | ASN A | 46150.513 | 13.691 | -7.944 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|---------|------|--------|
| ATOM | 644 | 1HB | ASN A | 46150.154 | 15.457 | - 9.891 | 1.00 | 0.00 H |
| ATOM | 645 | 2HB | ASN A | 46148.727 | 14.474 | -10.206 | 1.00 | 0.00 H |
| ATOM | 646 | 1HD2 | ASN A | 46150.433 | 15.953 | -7.468 | 1.00 | 0.00 H |
| ATOM | 647 | 2HD2 | ASN A | 46149.009 | 16.505 | -6.660 | 1.00 | 0.00 H |
| ATOM | 648 | N | GLU A | 47149.212 | 11.591 | -7.889 | 1.00 | 0.00 N |
| ATOM | 649 | CA | GLU A | 47148.370 | 10.404 | -7.789 | 1.00 | 0.00 C |
| ATOM | 650 | C | GLU A | 47148.235 | 9.958 | -6.339 | 1.00 | 0.00 C |
| ATOM | 651 | О | GLU A | 47149.230 | 9.655 | -5.679 | 1.00 | 0.00 O |
| ATOM | 652 | CB | GLU A | 47148.948 | 9.266 | -8.634 | 1.00 | 0.00 C |
| ATOM | 653 | CG | GLU A | 47150.467 | 9.182 | -8.595 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.033 | 8.332 | -9.715 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.096 | 8.825 | -10.861 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.415 | 7.173 | -9.446 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47149.752 | 11.859 | -7.117 | 1.00 | 0.00 H |
| ATOM | 658 | НА | GLU A | 47147.392 | 10.660 | -8.167 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.550 | 8.329 | -8.275 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47148.645 | 9.405 | -9.662 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47150.872 | 10.179 | -8.681 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47150.768 | 8.755 | -7.650 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.003 | 9.912 | -5.846 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VAL A | 48146.751 | 9.495 | -4.473 | 1.00 | 0.00 C |
| ATOM | 665 | C | VAL A | 48147.166 | 8.044 | -4.268 | 1.00 | 0.00 C |
| ATOM | 666 | O | VAL A | 48146.436 | 7.121 | -4.633 | 1.00 | 0.00 O |
| ATOM | 667 | CB | VAL A | 48145.266 | 9.655 | -4.096 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VAL A | 48145.057 | 9.375 | -2.616 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VALA | 48144.768 | 11.047 | -4.457 | 1.00 | 0.00 C |

| ATOM | 670 | Н | VAL A | 48146.248 | 10.161 | -6.418 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 671 | НА | VAL A | 48147.340 | 10.123 | -3.819 | 1.00 | 0.00 H |
| ATOM | 672 | НВ | VAL A | 48144.693 | 8.934 | -4.661 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48145.200 | 8.321 | -2.425 | 1.00 | 0.00 H |
| ATOM | 674 2 | 2HG1 | VAL A | 48144.055 | 9.659 | -2.334 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48145.769 | 9.945 | -2.037 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48145.443 | 11.500 | -5.168 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48144.724 | 11.656 | -3.566 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VAL A | 48143.783 | 10.975 | -4.893 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.343 | 7.846 | -3.684 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49148.856 | 6.506 | -3.434 | 1.00 | 0.00 C |
| ATOM | 681 | C | LEU A | 49148.772 | 6.164 | -1.953 | 1.00 | 0.00 C |
| ATOM | 682 | O | LEU A | 49149.439 | 6.784 | -1.124 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.304 | 6.392 | -3.915 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.503 | 6.575 | -5.421 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49151.948 | 6.937 | -5.729 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEU A | 49150.097 | 5.313 | -6.168 | 1.00 | 0.00 C |
| ATOM | 687 | Н | LEU A | 49148.880 | 8.621 | -3.416 | 1.00 | 0.00 H |
| ATOM | 688 | HA | LEU A | 49148.246 | 5.808 | -3.988 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49150.892 | 7.140 | -3.402 | 1.00 | 0.00 H |
| ATOM | 690 2 | 2HB | LEU A | 49150.677 | 5.416 | -3.642 | 1.00 | 0.00 H |
| ATOM | 691 | HG | LEU A | 49149.875 | 7.384 | -5.765 | 1.00 | 0.00 H |
| ATOM | 692 | 1HD1 | LEU A | 49151.984 | 7.547 | -6.619 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49152.519 | 6.035 | -5.886 | 1.00 | 0.00 H |
| ATOM | 694 | 3HD1 | LEU A | 49152.366 | 7.487 | -4.898 | 1.00 | 0.00 H |
| ATOM | 695 | 1HD2 | LEU A | 49149.362 | 4.774 | -5.589 | 1.00 | 0.00 H |
| ATOM | 696 | 2HD2 | LEU A | 49150.966 | 4.689 | -6.318 | 1.00 | 0.00 H |

| ATOM | 697 | 3HD2 | LEU A | 49149.676 | 5.581 | -7.125 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 698 | N | ALA A | 50147.948 | 5.176 | -1.625 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.780 | 4.758 | -0.242 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALA A | 50148.746 | 3.631 | 0.112 | 1.00 | 0.00 C |
| ATOM | 701 | О | ALA A | 50148.657 | 2.531 | -0.433 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.342 | 4.325 | 0.007 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.443 | 4.719 | -2.329 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50147.989 | 5.610 | 0.387 | 1.00 | 0.00 H |
| ATOM | 705 | IНВ | ALA A | 50145.712 | 4.691 | -0.789 | 1.00 | 0.00 H |
| ATOM | 706 2 | 2HB | ALA A | 50146.003 | 4.728 | 0.949 | 1.00 | 0.00 H |
| ATOM | 707 3 | ВНВ | ALA A | 50146.292 | 3.246 | 0.039 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.668 | 3.914 | 1.025 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.637 | 2.915 | 1.434 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51150.011 | 1.789 | 2.232 | 1.00 | 0.00 C |
| ATOM | 711 | О | GLY A | 51149.679 | 1.961 | 3.406 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.691 | 4.808 | 1.425 | 1.00 | 0.00 H |
| ATOM | 713 | 1HA | GLY A | 51151.104 | 2.499 | 0.553 | 1.00 | 0.00 H |
| ATOM | 714 2 | 2HA | GLY A | 51151.396 | 3.391 | 2.039 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.848 | 0.634 | 1.596 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.257 | -0.524 | 2.256 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.331 | -1.381 | 2.919 | 1.00 | 0.00 C |
| ATOM | 718 | O | LEU A | 52151.450 | -1.488 | 2.418 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.468 | -1.365 | 1.248 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.201 | -0.702 | 0.703 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.592 | -1.549 | -0.403 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52146.196 | -0.478 | 1.823 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.133 | 0.558 | 0.662 | 1.00 | 0.00 H |

| ATOM | 724 | НА | LEU A | 52148.581 | -0.163 | 3.016 | 1.00 | 0.00 H |
|--------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 725 | 1HB | LEU A | 52149.119 | -1.592 | 0.416 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52148.187 | -2.291 | 1.726 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.458 | 0.260 | 0.284 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52146.403 | -2.546 | -0.032 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52147.276 | -1.599 | -1.237 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52145.663 | -1.103 | -0.726 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52146.362 | -1.202 | 2.607 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52145.194 | -0.592 | 1.434 | 1.00 | 0.00 H |
| ATOM · | 733 | 3HD2 | LEU A | 52146.316 | 0.519 | 2.220 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53149.982 | -1.988 | 4.049 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.916 | -2.836 | 4.781 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.448 | -4.287 | 4.782 | 1.00 | 0.00 C |
| ATOM | 737 | Ο | GLU A | 53149.515 | -4.649 | 5.499 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.069 | -2.336 | 6.219 | 1.00 | 0.00 C |
| ATOM | 739 | CG | GLU A | 53152.057 | -3.146 | 7.042 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.571 | -3.395 | 8.457 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53151.282 | -4.563 | 8.789 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53151.482 | -2.420 | 9.234 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53149.075 | -1.864 | 4.398 | 1.00 | 0.00 H |
| ATOM | 744 | НА | GLU A | 53151.874 | -2.779 | 4.286 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.407 | -1.311 | 6.198 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53150.107 | -2.379 | 6.707 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53152.212 | -4.099 | 6.560 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53152.994 | -2.610 | 7.088 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54151.103 | -5.114 | 3.974 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.754 | -6.527 | 3.881 | 1.00 | 0.00 C |

| ATOM | 751 | C | LEU A | 54151.046 | -7.247 | 5.194 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|---------|--------|------|--------|
| ATOM | 752 | О | LEU A | 54152.057 | -6.982 | 5.846 | 1.00 | 0.00 O |
| ATOM | 753 | СВ | LEU A | 54151.524 | -7.191 | 2.739 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.324 | -6.552 | 1.364 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.297 | -7.140 | 0.354 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54149.889 | -6.740 | 0.895 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.838 | -4.767 | 3.426 | 1.00 | 0.00 H |
| ATOM | 758 | НА | LEU A | 54149.696 | -6.594 | 3.676 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.578 | -7.160 | 2.978 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54151.219 | -8.225 | 2.679 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.517 | -5.492 | 1.435 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54152.308 | -8.216 | 0.449 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54153.288 | -6.753 | 0.542 | 1.00 | 0.00 H |
| ATOM | 764 | 3HD1 | LEU A | 54151.988 | -6.870 | -0.644 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54149.541 | -7.721 | 1.183 | 1.00 | 0.00 H |
| ATOM | 766 | 2HD2 | LEU A | 54149.846 | -6.644 | -0.180 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.260 | -5.988 | 1.349 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55150.156 | -8.157 | 5.576 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55150.320 | -8.914 | 6.811 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55151.395 | -9.986 | 6.655 | 1.00 | 0.00 C |
| ATOM | 771 | О | GLU A | 55152.090 | -10.325 | 7.612 | 1.00 | 0.00 O |
| ATOM | 772 | СВ | GLU A | 55148.994 | -9.562 | 7.217 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55147.871 | -8.562 | 7.436 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55147.824 | -8.042 | 8.859 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55146.921 | -8.458 | 9.615 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55148.691 | - 7.217 | 9.219 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.372 | -8.323 | 5.014 | 1.00 | 0.00 H |

| ATOM | 778 | HA | GLU A | 55150.625 | -8.225 | 7.584 | 1.00 | 0.00 H |
|------|---------------|-----|-------|--------------|---------|-------|------|--------|
| ATOM | 779 | lНВ | GLU A | 55148.689 - | 10.248 | 6.441 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55149.142 - | 10.112 | 8.134 | 1.00 | 0.00 H |
| ATOM | 78 1 1 | lHG | GLU A | 55148.015 | -7.726 | 6.769 | 1.00 | 0.00 H |
| ATOM | 782 2 | 2HG | GLU A | 55146.930 | -9.042 | 7.213 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56151.525 -1 | 10.513 | 5.442 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASP A | 56152.516 - | 11.547 | 5.161 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASPA | 56153.811 -1 | 0.931 | 4.642 | 1.00 | 0.00 C |
| ATOM | 786 | О | ASPA | 56153.807 -1 | 10.183 | 3.665 | 1.00 | 0.00 O |
| ATOM | 787 | CB | ASPA | 56151.967 - | 12.544 | 4.140 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56152.412 - | 13.965 | 4.423 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASPA | 56153.373 -1 | 4.428 | 3.773 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56151.800 -1 | 4.618 | 5.295 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.941 -1 | 10.202 | 4.719 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.723 - | 12.067 | 6.085 | 1.00 | 0.00 H |
| ATOM | 793 1 | lНВ | ASPA | 56150.887 -1 | 2.516 | 4.162 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASP A | 56152.310 -1 | 2.268 | 3.155 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.919 - | 11.252 | 5.303 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57156.222 - | -10.731 | 4.908 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.628 - | 11.260 | 3.536 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57157.106 - | 12.388 | 3.411 | 1.00 | 0.00 O |
| ATOM | 799 | СВ | GLU A | 57157.282 - | -11.108 | 5.946 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.377 | -10.126 | 7.102 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57158.593 | -10.371 | 7.975 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57158.766 - | 11.514 | 8.445 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57159.372 | -9.418 | 8.188 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.858 - | 11.854 | 6.074 | 1.00 | 0.00 H |

| ATOM | 805 | HA | GLU A | 57156.148 | -9.655 | 4.858 | 1.00 | 0.00 H |
|-------------------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 806 | lНВ | GLU A | 57157.044 | 12.082 | 6.347 | 1.00 | 0.00 H |
| ATOM | 807 2 | 2HB | GLU A | 57158.245 | -11.154 | 5.460 | 1.00 | 0.00 H |
| ATOM | 808 | HG | GLU A | 57157.436 | -9.124 | 6.703 | 1.00 | 0.00 H |
| ATOM | 809 2 | 2HG | GLU A | 57156.490 | -10.219 | 7.711 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58156.432 - | 10.439 | 2.510 | 1.00 | 0.00 N |
| ATOM [*] | 811 | CA | CYS A | 58156.777 | -10.825 | 1.146 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58158.157 - | 10.301 | 0.765 | 1.00 | 0.00 C |
| ATOM | 813 | O | CYS A | 58158.426 | -9.103 | 0.859 | 1.00 | 0.00 O |
| ATOM | 814 | СВ | CYS A | 58155.730 | -10.297 | 0.164 | 1.00 | 0.00 C |
| ATOM | 815 | SG | CYSA | 58155.833 | -11.026 | -1.487 | 1.00 | 0.00 S |
| ATOM | 816 | Н | CYS A | 58156.047 | -9.553 | 2.673 | 1.00 | 0.00 H |
| ATOM | 817 | НА | CYS A | 58156.789 | -11.903 | 1.100 | 1.00 | 0.00 H |
| ATOM | 818 | IНВ | CYS A | 58154.745 - | 10.506 | 0.553 | 1.00 | 0.00 H |
| ATOM | 819 2 | 2HB | CYS A | 58155.851 | -9.229 | 0.060 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYS A | 58155.366 | -10.449 | -2.096 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALA A | 59159.031 | -11.207 | 0.335 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALA A | 59160.383 | -10.836 | -0.060 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59160.374 | 10.001 | -1.337 | 1.00 | 0.00 C |
| ATOM | 824 | О | ALA A | 59160.036 | -10.496 | -2.411 | 1.00 | 0.00 O |
| ATOM | 825 | CB | ALAA | 59161.238 | -12.081 | -0.249 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALA A | 59158.758 | -12.146 | 0.282 | 1.00 | 0.00 H |
| ATOM | 827 | HA | ALA A | 59160.815 | -10.250 | 0.738 | 1.00 | 0.00 H |
| ATOM | 828 | lНВ | ALA A | 59161.020 | 12.524 | -1.210 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59161.015 | 12.792 | 0.533 | 1.00 | 0.00 H |
| ATOM | 830 3 | ЗНВ | ALA A | 59162.282 | -11.811 | -0.205 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60160.746 | -8.732 | -1.209 | 1.00 | 0.00 N |

| ATOM | 832 | CA | GLY A | 60160.773 | -7.848 | -2.360 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 833 | C | GLY A | 60160.174 | -6.487 | -2.062 | 1.00 | 0.00 C |
| ATOM | 834 | О | GLY A | 60160.550 | -5.488 | -2.673 | 1.00 | O.00 O |
| ATOM | 835 | Н | GLY A | 60161.005 | -8.392 | -0.328 | 1.00 | 0.00 H |
| ATOM | 836 | IHA | GLY A | 60161.797 | -7.717 | -2.677 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60160.215 | -8.306 | -3.165 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61159.239 | -6.449 | -1.118 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.586 | -5.201 | -0.739 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.505 | -4.349 | 0.132 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.621 | -4.755 | 0.456 | 1.00 | 0.00 O |
| ATOM | 842 | СВ | CYS A | 61157.281 | -5.490 | 0.005 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYS A | 61156.114 | -6.515 | -0.920 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.981 | -7.280 | -0.667 | 1.00 | 0.00 H |
| ATOM | 845 | НА | CYS A | 61158.361 | -4.657 | -1.644 | 1.00 | 0.00 H |
| ATOM | 846 | lНВ | CYS A | 61157.507 | -6.002 | 0.928 | 1.00 | 0.00 H |
| ATOM | 847 2 | 2HB | CYS A | 61156.791 | -4.554 | 0.230 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61155.351 | -6.675 | -0.360 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62159.026 | -3.168 | 0.508 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.805 | -2.260 | 1.342 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.217 | -2.171 | 2.746 | 1.00 | 0.00 C |
| ATOM | 852 | O | THR A | 62158.231 | -2.839 | 3.059 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62159.854 | -0.868 | 0.708 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.550 | -0.421 | 0.380 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.689 | -0.814 | -0.553 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62158.130 | -2.901 | 0.218 | 1.00 | 0.00 H |
| ATOM | 857 | HA | THR A | 62160.810 | -2.650 | 1.410 | 1.00 | 0.00 H |
| ATOM | 858 | НВ | THR A | 62160.282 | -0.176 | 1.418 | 1.00 | 0.00 H |

| ATOM | 859 | HG1 | THR A | 62158.188 | -0.974 | -0.315 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 860 | 1HG2 | THR A | 62160.904 | -1.819 | -0.886 | 1.00 | 0.00 H |
| ATOM | 861 2 | 2HG2 | THR A | 62161.615 | -0.296 | -0.349 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62160.144 | -0.288 | -1.323 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63159.827 | -1.342 | 3.587 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASP A | 63159.363 | -1.166 | 4.958 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.671 | 0.182 | 5.130 | 1.00 | 0.00 C |
| ATOM | 866 | О | ASPA | 63158.779 | 0.818 | 6.178 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASPA | 63160.536 | -1.278 | 5.934 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.601 | -0.229 | 5.680 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63162.691 | -0.596 | 5.192 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63161.345 | 0.958 | 5.968 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASPA | 63160.608 | -0.838 | 3.278 | 1.00 | 0.00 H |
| ATOM | 872 | НА | ASPA | 63158.653 | -1.952 | 5.171 | 1.00 | 0.00 H |
| ATOM | 873 | 1HB | ASPA | 63160.170 | -1.156 | 6.942 | 1.00 | 0.00 H |
| ATOM | 874 | 2HB | ASPA | 63160.987 | -2.255 | 5.834 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64157.960 | 0.612 | 4.093 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.260 | 1.882 | 4.148 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64158.013 | 2.990 | 3.440 | 1.00 | 0.00 C |
| ATOM | 878 | О | GLY A | 64158.125 | 4.102 | 3.956 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64157.909 | 0.062 | 3.282 | 1.00 | 0.00 H |
| ATOM | 880 | 1HA | GLY A | 64156.291 | 1.767 | 3.687 | 1.00 | 0.00 H |
| ATOM | 881 2 | 2HA | GLY A | 64157.123 | 2.160 | 5.183 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.529 | 2.687 | 2.253 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.276 | 3.667 | 1.472 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65158.845 | 3.638 | 0.009 | 1.00 | 0.00 C |
| ATOM | 885 | O | THR A | 65158.797 | 2.578 | -0.614 | 1.00 | 0.00 O |

| ATOM | 886 | CB | THR A | 65160.778 | 3.398 | 1.578 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|-------|---------|------|--------|
| ATOM | 887 | OG1 | THR A | 65161.034 | 2.006 | 1.641 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.415 | 4.039 | 2.791 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.406 | 1.784 | 1.894 | 1.00 | 0.00 H |
| ATOM | 890 | НА | THR A | 65159.064 | 4.645 | 1.877 | 1.00 | 0.00 H |
| ATOM | 891 | НВ | THR A | 65161.266 | 3.793 | 0.700 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65160.910 | 1.618 | 0.773 | 1.00 | 0.00 H |
| ATOM | 893 | 1HG2 | THR A | 65162.234 | 3.423 | 3.135 | 1.00 | 0.00 H |
| ATOM | 894 | 2HG2 | THR A | 65160.681 | 4.133 | 3.577 | 1.00 | 0.00 H |
| ATOM | 895 | 3HG2 | THR A | 65161.788 | 5.018 | 2.527 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.530 | 4.811 | -0.533 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.103 | 4.921 | -1.923 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.010 | 5.872 | -2.697 | 1.00 | 0.00 C |
| ATOM | 899 | О | PHE A | 66159.157 | 7.039 | -2.334 | 1.00 | 0.00 O |
| ATOM | 900 | CB | PHE A | 66156.655 | 5.406 | - 1.996 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66155.978 | 5.083 | -3.298 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.722 | 3.769 | -3.654 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.598 | 6.094 | -4.166 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.100 | 3.468 | -4.851 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66154.976 | 5.801 | -5.364 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.726 | 4.486 | -5.707 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.588 | 5.621 | 0.015 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66158.168 | 3.939 | -2.369 | 1.00 | 0.00 H |
| ATOM | 909 | 1HB | PHE A | 66156.086 | 4.943 | -1.204 | 1.00 | 0.00 H |
| ATOM | 910 | 2HB | PHE A | 66156.635 | 6.478 | -1.867 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66156.014 | 2.973 | -2.985 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66155.792 | 7.123 | -3.898 | 1.00 | 0.00 H |
| | | | | | | | | |

| ATOM | 913 | HE1 | PHE A | 66154.907 | 2.440 | -5.117 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|---------|------|--------|
| ATOM | 914 | HE2 | PHE A | 66154.684 | 6.598 | -6.032 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.240 | 4.254 | -6.643 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.615 | 5.366 | -3.767 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67160.508 | 6.172 | -4.592 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.689 | 6.684 | -3.776 | 1.00 | 0.00 C |
| ATOM | 919 | О | ARG A | 67162.217 | 7.765 | -4.039 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67159.746 | 7.348 | -5.204 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67158.677 | 6.930 | -6.200 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67158.317 | 8.067 | -7.143 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67159.015 | 7.958 | -8.422 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67159.160 | 8.970 | -9.274 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67158.658 | 10.165 | -8.989 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67159.808 | 8.786 - | -10.417 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.458 | 4.429 | -4.006 | 1.00 | 0.00 H |
| ATOM | 928 | НА | ARG A | 67160.881 | 5.543 | -5.387 | 1.00 | 0.00 H |
| ATOM | 929 1 | НВ | ARG A | 67159.271 | 7.906 | -4.411 | 1.00 | 0.00 H |
| ATOM | 930 2 | HB | ARG A | 67160.449 | 7.991 | -5.714 | 1.00 | 0.00 H |
| ATOM | 931 1 | HG | ARG A | 67159.045 | 6.097 | -6.780 | 1.00 | 0.00 H |
| ATOM | 932 2 | HG | ARG A | 67157.792 | 6.629 | -5.657 | 1.00 | 0.00 H |
| ATOM | 933 1 | HD | ARG A | 67157.253 | 8.045 | -7.322 | 1.00 | 0.00 H |
| ATOM | 934 2 | 2HD | ARG A | 67158.585 | 9.003 | -6.675 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67159.396 | 7.087 | -8.657 | 1.00 | 0.00 H |
| ATOM | 936 1 | HH1 | ARG A | 67158.168 | 10.311 | -8.129 | 1.00 | 0.00 H |
| ATOM | 937 2 | HH1 | ARG A | 67158.771 | 10.921 | -9.634 | 1.00 | 0.00 H |
| ATOM | 938 1 | нн2 | ARG A | 67160.188 | 7.888 - | 10.637 | 1.00 | 0.00 H |
| ATOM | 939 2 | нн2 | ARG A | 67159.917 | 9.546 - | 11.058 | 1.00 | 0.00 H |

| ATOM | 940 | N | GLY A | 68162.100 | 5.902 | -2.783 | 1.00 | 0.00 N |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 941 | CA | GLY A | 68163.216 | 6.295 | -1.942 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.847 | 7.392 | -0.963 | 1.00 | 0.00 C |
| ATOM | 943 | О | GLY A | 68163.696 | 8.189 | -0.564 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68161.641 | 5.052 | -2.619 | 1.00 | 0.00 H |
| ATOM | 945 | 1HA | GLY A | 68163.556 | 5.433 | -1.389 | 1.00 | 0.00 H |
| ATOM | 946 | 2HA | GLY A | 68164.020 | 6.645 | -2.572 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.577 | 7.433 | -0.576 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69161.096 | 8.441 | 0.363 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69160.235 | 7.806 | 1.449 | 1.00 | 0.00 C |
| ATOM | 950 | Ο | THR A | 69159.141 | 7.310 | 1.178 | 1.00 | 0.00 O |
| ATOM | 951 | CB | THR A | 69160.297 | 9.515 | -0.375 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.987 | 9.948 | -1.533 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69160.010 | 10.737 | 0.472 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.947 | 6.771 | -0.928 | 1.00 | 0.00 H |
| ATOM | 955 | HA | THR A | 69161.957 | 8.900 | 0.825 | 1.00 | 0.00 H |
| ATOM | 956 | HB | THR A | 69159.349 | 9.096 | -0.682 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.176 | 9.193 | -2.095 | 1.00 | 0.00 H |
| ATOM | 958 | 1HG2 | THR A | 69159.249 | 11.336 | -0.006 | 1.00 | 0.00 H |
| ATOM | 959 | 2HG2 | THR A | 69160.913 | 11.319 | 0.579 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69159.665 | 10.425 | 1.447 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.735 | 7.825 | 2.680 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70160.011 | 7.251 | 3.809 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.731 | 8.032 | 4.087 | 1.00 | 0.00 C |
| ATOM | 964 | O | ARG A | 70158.765 | 9.242 | 4.308 | 1.00 | 0.00 O |
| ATOM | 965 | CB | ARG A | 70160.897 | 7.239 | 5.057 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70160.228 | 6.616 | 6.272 | 1.00 | 0.00 C |

| ATOM | 967 | CD | ARG A | 70160.684 | 7.279 | 7.561 | 1.00 | 0.00 C |
|------|-------|-------|-------|-----------|--------|--------|------|--------|
| ATOM | 968 | NE | ARG A | 70162.045 | 6.890 | 7.924 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70162.802 | 7.562 | 8.789 | 1.00 | 0.00 C |
| ATOM | 970 | NH1 | ARG A | 70162.336 | 8.654 | 9.381 | 1.00 | 0.00 N |
| ATOM | 971 | NH2 | ARG A | 70164.028 | 7.139 | 9.064 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.612 | 8.235 | 2.834 | 1.00 | 0.00 H |
| ATOM | 973 | HA | ARG A | 70159.751 | 6.235 | 3.553 | 1.00 | 0.00 H |
| ATOM | 974 | lНВ | ARG A | 70161.795 | 6.681 | 4.842 | 1.00 | 0.00 H |
| ATOM | 975 2 | 2HB | ARG A | 70161.166 | 8.256 | 5.303 | 1.00 | 0.00 H |
| ATOM | 976 | IHG | ARG A | 70159.158 | 6.731 | 6.180 | 1.00 | 0.00 H |
| ATOM | 977 2 | 2HG | ARG A | 70160.477 | 5.566 | 6.309 | 1.00 | 0.00 H |
| ATOM | 978 | HD | ARG A | 70160.650 | 8.351 | 7.431 | 1.00 | 0.00 H |
| ATOM | 979 2 | 2HD | ARG A | 70160.013 | 6.992 | 8.356 | 1.00 | 0.00 H |
| ATOM | 980 | HE | ARG A | 70162.414 | 6.086 | 7.502 | 1.00 | 0.00 H |
| ATOM | 981 | IHHI. | ARG A | 70161.412 | 8.979 | 9.178 | 1.00 | 0.00 H |
| ATOM | 982 2 | 2HH1. | ARG A | 70162.909 | 9.154 | 10.030 | 1.00 | 0.00 H |
| ATOM | 983 | HH2 | ARG A | 70164.384 | 6.316 | 8.621 | 1.00 | 0.00 H |
| ATOM | 984 2 | 2HH2. | ARG A | 70164.597 | 7.643 | 9.714 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.602 | 7.330 | 4.076 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71156.310 | 7.957 | 4.327 | 1.00 | 0.00 C |
| ATOM | 987 | C | TYR A | 71155.770 | 7.560 | 5.696 | 1.00 | 0.00 C |
| ATOM | 988 | О | TYR A | 71155.270 | 8.400 | 6.446 | 1.00 | 0.00 O |
| ATOM | 989 | СВ | TYR A | 71155.309 | 7.566 | 3.238 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.424 | 8.400 | 1.981 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.529 | 9.784 | 2.050 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.426 | 7.802 | 0.727 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.635 | 10.548 | 0.905 | 1.00 | 0.00 C |

| ATOM | 994 | CE2 | TYR A | 71155.532 | 8.561 | -0.424 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 995 | CZ | TYR A | 71155.635 | 9.933 | -0.330 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71155.740 | 10.691 | -1.473 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.639 | 6.368 | 3.893 | 1.00 | 0.00 H |
| ATOM | 998 | НА | TYR A | 71156.451 | 9.028 | 4.306 | 1.00 | 0.00 H |
| ATOM | 999 1 | НВ | TYR A | 71155.468 | 6.533 | 2.966 | 1.00 | 0.00 H |
| ATOM | 1000 2 | 2HB | TYR A | 71154.306 | 7.681 | 3.623 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.529 | 10.262 | 3.018 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.344 | 6.728 | 0.657 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.716 | 11.623 | 0.978 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.531 | 8.078 | -1.390 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71156.629 | 10.616 | -1.827 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72155.873 | 6.274 | 6.017 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.395 | 5.765 | 7.298 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.315 | 4.669 | 7.825 | 1.00 | 0.00 C |
| ATOM | 1009 | O | PHE A | 72157.106 | 4.095 | 7.077 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72153.969 | 5.226 | 7.156 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72153.833 | 4.157 | 6.110 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72153.929 | 2.818 | 6.453 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72153.609 | 4.491 | 4.785 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72153.804 | 1.832 | 5.493 | 1.00 | 0.00 C |
| ATOM | 1015 | CE2 | PHE A | 72153.483 | 3.510 | 3.820 | 1.00 | 0.00 C |
| ATOM | 1016 | CZ | PHE A | 72153.581 | 2.178 | 4.174 | 1.00 | 0.00 C |
| ATOM | 1017 | Н | PHE A | 72156.281 | 5.653 | 5.379 | 1.00 | 0.00 H |
| ATOM | 1018 | HA | PHE A | 72155.392 | 6.585 | 8.001 | 1.00 | 0.00 H |
| ATOM | 1019 | HB | PHE A | 72153.655 | 4.809 | 8.101 | 1.00 | 0.00 H |
| ATOM | 1020 2 | 2HB | PHE A | 72153.311 | 6.039 | 6.890 | 1.00 | 0.00 H |

| ATOM | 1021 | HD1 | PHE A | 72154.104 | 2.546 | 7.484 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1022 | HD2 | PHE A | 72153.533 | 5.532 | 4.507 | 1.00 | 0.00 H |
| ATOM | 1023 | HE1 | PHE A | 72153.881 | 0.792 | 5.773 | 1.00 | 0.00 H |
| ATOM | 1024 | HE2 | PHE A | 72153.309 | 3.784 | 2.789 | 1.00 | 0.00 H |
| ATOM | 1025 | HZ | PHE A | 72153.483 | 1.410 | 3.423 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73156.207 | 4.384 | 9.119 | 1.00 | 0.00 N |
| ATOM | 1027 | CA | THR A | 73157.029 | 3.357 | 9.747 | 1.00 | 0.00 C |
| ATOM | 1028 | C | THR A | 73156.250 | 2.054 | 9.899 | 1.00 | 0.00 C |
| ATOM | 1029 | O | THR A | 73155.248 | 1.997 | 10.611 | 1.00 | 0.00 O |
| ATOM | 1030 | CB | THR A | 73157.520 | 3.832 | 11.114 | 1.00 | 0.00 C |
| ATOM | 1031 | OG1 | THR A | 73156.507 | 4.562 | 11.785 | 1.00 | 0.00 O |
| ATOM | 1032 | CG2 | THR A | 73158.746 | 4.716 | 11.036 | 1.00 | 0.00 C |
| ATOM | 1033 | Н | THR A | 73155.558 | 4.877 | 9.665 | 1.00 | 0.00 H |
| ATOM | 1034 | НА | THR A | 73157.882 | 3.180 | 9.110 | 1.00 | 0.00 H |
| ATOM | 1035 | НВ | THR A | 73157.771 | 2.969 | 11.716 | 1.00 | 0.00 H |
| ATOM | 1036 | HG1 | THR A | 73156.474 | 4.291 | 12.706 | 1.00 | 0.00 H |
| ATOM | 1037 | HG2 | THR A | 73159.529 | 4.199 | 10.501 | 1.00 | 0.00 H |
| ATOM | 1038 2 | 2HG2 | THR A | 73159.086 | 4.949 | 12.034 | 1.00 | 0.00 H |
| ATOM | 1039 3 | 3HG2 | THR A | 73158.498 | 5.630 | 10.517 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYS A | 74156.717 | 1.009 | 9.222 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74156.065 | -0.294 | 9.281 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74157.095 | -1.417 | 9.320 | 1.00 | 0.00 C |
| ATOM | 1043 | O | CYSA | 74158.301 | -1.169 | 9.289 | 1.00 | 0.00 O |
| ATOM | 1044 | CB | CYS A | 74155.136 | -0.478 | 8.080 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYSA | 74153.445 | 0.096 | 8.360 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYS A | 74157.521 | 1.117 | 8.670 | 1.00 | 0.00 H |
| ATOM | 1047 | HA | CYS A | 74155.478 | -0.329 | 10.188 | 1.00 | 0.00 H |

ATOM 1048 1HB CYS A 74155.534 0.072 0.00 H 7.241 1.00 **ATOM** 1049 2HB CYS A -1.5270.00 H 74155.091 7.828 1.00 **ATOM** 1050 HG CYS A 74153.194 0.00 H -0.1479.254 1.00 1051 N 75156.613 1.00 0.00 N **ATOM ALAA** -2.654 9.386 **ATOM** 1052 $\mathsf{C}\mathsf{A}$ **ALAA** 75157.492 -3.816 9.428 1.00 0.00 C 1053 C 75158.208 8.096 1.00 0.00 C **ATOM ALAA** -4.011 1054 75157.739 1.00 0.00 O **ATOM** 0 **ALAA** -3.552 7.055 **ATOM** 1055 CB **ALAA** 75156.700 -5.062 9.791 1.00 0.00 C 1056 Η 75155.642 -2.787 1.00 0.00 H **ATOM ALAA** 9.407 75158.229 1.00 **ATOM** 1057 HA **ALAA** -3.648 10.200 0.00 H **ATOM** 1058 1HB **ALAA** 75157.137 -5.921 9.302 1.00 0.00 H 75155.676 -4.945 9.467 1.00 0.00 H **ATOM** 1059 2HB **ALAA** 10.861 1.00 0.00 H **ATOM** 1060 3HB **ALAA** 75156.725 -5.206 76159.347 8.137 1.00 0.00 N **ATOM** 1061 N LEU A -4.695 CA LEU A 76160.129 -4.952 6.933 1.00 0.00 C **ATOM** 1062 **ATOM** 1063 \mathbf{C} LEU A 76159.419 -5.953 6.027 1.00 0.00 C LEU A 76158.846 **ATOM** 1064 O -6.9346.499 1.00 0.00 O 1065 -5.476 7.303 1.00 0.00 C **ATOM** CB LEU A 76161.518 **ATOM** 1066 CG LEUA 76162.487 -4.420 7.837 1.00 0.00 C CD1 LEU A 76163.413 -5.024 8.882 1.00 0.00 C **ATOM** 1067 CD2 LEU A 76163.291 -3.8126.698 1.00 0.00 C **ATOM** 1068 8.997 LEU A 76159.669 -5.036 1.00 0.00 H **ATOM** 1069 Η HA LEUA 76160.236 -4.017 6.402 1.00 0.00 H **ATOM** 1070 1071 1HB LEU A 76161.401 -6.242 8.056 1.00 0.00 H **ATOM** 6.425 1.00 0.00 H 1072 2HB LEU A 76161.956 -5.923 **ATOM** 8.309 1.00 0.00 H1073 HG LEUA 76161.923 -3.629**ATOM** 0.00 H 1.00 **ATOM** 1074 1HD1 LEU A 76163.579 -6.067 8.655

| ATOM | 1075 2HD1 | LEU A | 76162.961 | -4.934 | 9.858 | 1.00 | 0.00 H |
|------|-----------|-------|-----------|--------|-------|------|--------|
| ATOM | 1076 3HD1 | LEU A | 76164.357 | -4.499 | 8.873 | 1.00 | 0.00 H |
| ATOM | 1077 1HD2 | LEU A | 76162.802 | -2.913 | 6.350 | 1.00 | 0.00 H |
| ATOM | 1078 2HD2 | LEU A | 76163.359 | -4.522 | 5.886 | 1.00 | 0.00 H |
| ATOM | 1079 3HD2 | LEU A | 76164.284 | -3.568 | 7.046 | 1.00 | 0.00 H |
| ATOM | 1080 N | LYSA | 77159.463 | -5.699 | 4.723 | 1.00 | 0.00 N |
| ATOM | 1081 CA | LYS A | 77158.826 | -6.579 | 3.751 | 1.00 | 0.00 C |
| ATOM | 1082 C | LYS A | 77157.321 | -6.654 | 3.991 | 1.00 | 0.00 C |
| ATOM | 1083 O | LYSA | 77156.714 | -7.719 | 3.867 | 1.00 | 0.00 O |
| ATOM | 1084 CB | LYS A | 77159.436 | -7.980 | 3.821 | 1.00 | 0.00 C |
| ATOM | 1085 CG | LYS A | 77160.953 | -7.988 | 3.712 | 1.00 | 0.00 C |
| ATOM | 1086 CD | LYS A | 77161.411 | -7.675 | 2.296 | 1.00 | 0.00 C |
| ATOM | 1087 CE | LYS A | 77162.908 | -7.415 | 2.240 | 1.00 | 0.00 C |
| ATOM | 1088 NZ | LYS A | 77163.667 | -8.625 | 1.820 | 1.00 | 0.00 N |
| ATOM | 1089 H | LYS A | 77159.937 | -4.902 | 4.408 | 1.00 | 0.00 H |
| ATOM | 1090 HA | LYS A | 77159.002 | -6.168 | 2.768 | 1.00 | 0.00 H |
| ATOM | 1091 1HB | LYS A | 77159.163 | -8.433 | 4.762 | 1.00 | 0.00 H |
| ATOM | 1092 2HB | LYS A | 77159.036 | -8.576 | 3.014 | 1.00 | 0.00 H |
| ATOM | 1093 1HG | LYS A | 77161.357 | -7.245 | 4.383 | 1.00 | 0.00 H |
| ATOM | 1094 2HG | LYS A | 77161.319 | -8.966 | 3.991 | 1.00 | 0.00 H |
| ATOM | 1095 1HD | LYS A | 77161.177 | -8.513 | 1.658 | 1.00 | 0.00 H |
| ATOM | 1096 2HD | LYS A | 77160.888 | -6.797 | 1.945 | 1.00 | 0.00 H |
| ATOM | 1097 1HE | LYS A | 77163.096 | -6.620 | 1.534 | 1.00 | 0.00 H |
| ATOM | 1098 2HE | LYS A | 77163.244 | -7.112 | 3.221 | 1.00 | 0.00 H |
| ATOM | 1099 1HZ | LYS A | 77163.116 | -9.483 | 2.031 | 1.00 | 0.00 H |
| ATOM | 1100 2HZ | LYS A | 77164.572 | -8.674 | 2.329 | 1.00 | 0.00 H |
| ATOM | 1101 3HZ | LYS A | 77163.857 | -8.590 | 0.798 | 1.00 | 0.00 H |

| ATOM | 1102 | N | LYS A | 78156.724 | -5.518 | 4.334 | 1.00 | 0.00 N |
|------|--------|-----|-------|-----------|--------|-------|------|--------|
| ATOM | 1103 | CA | LYS A | 78155.290 | -5.455 | 4.591 | 1.00 | 0.00 C |
| ATOM | 1104 | C | LYS A | 78154.730 | -4.086 | 4.219 | 1.00 | 0.00 C |
| ATOM | 1105 | О | LYS A | 78153.888 | -3.534 | 4.928 | 1.00 | 0.00 O |
| ATOM | 1106 | СВ | LYS A | 78155.001 | -5.755 | 6.063 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.529 | -7.104 | 6.524 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYSA | 78155.130 | -7.398 | 7.961 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYSA | 78153.930 | -8.331 | 8.026 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78152.998 | -7.961 | 9.126 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.261 | -4.702 | 4.417 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.811 | -6.205 | 3.980 | 1.00 | 0.00 H |
| ATOM | 1113 1 | НВ | LYS A | 78155.457 | -4.988 | 6.671 | 1.00 | 0.00 H |
| ATOM | 11142 | 2HB | LYS A | 78153.932 | -5.739 | 6.219 | 1.00 | 0.00 H |
| ATOM | 1115 1 | HG | LYS A | 78155.126 | -7.875 | 5.884 | 1.00 | 0.00 H |
| ATOM | 11162 | 2HG | LYS A | 78156.607 | -7.101 | 6.452 | 1.00 | 0.00 H |
| ATOM | 1117 1 | HD | LYS A | 78155.962 | -7.864 | 8.468 | 1.00 | 0.00 H |
| ATOM | 1118 2 | 2HD | LYS A | 78154.879 | -6.470 | 8.452 | 1.00 | 0.00 H |
| ATOM | 1119 1 | HE | LYS A | 78153.401 | -8.283 | 7.086 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYSA | 78154.283 | -9.339 | 8.188 | 1.00 | 0.00 H |
| ATOM | 1121 | ΙHZ | LYS A | 78152,591 | -8.817 | 9.553 | 1.00 | 0.00 H |
| ATOM | 1122 2 | 2HZ | LYS A | 78152.225 | -7.371 | 8.757 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYS A | 78153.505 | -7.426 | 9.860 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.202 | -3.543 | 3.101 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.749 | -2.238 | 2.635 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.591 | -2.223 | 1.118 | 1.00 | 0.00 C |
| ATOM | 1127 | О | ALA A | 79155.576 | -2.254 | 0.381 | 1.00 | 0.00 O |
| ATOM | 1128 | СВ | ALA A | 79155.718 | -1.153 | 3.077 | 1.00 | 0.00 C |

| ATOM | 1129 | Н | ALA A | 79155.872 | -4.031 | 2.578 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1130 | НА | ALA A | 79153.789 | -2.038 | 3.088 | 1.00 | 0.00 H |
| ATOM | 1131 | 1HB | ALA A | 79155.189 | -0.216 | 3.177 | 1.00 | 0.00 H |
| ATOM | 1132 | 2HB | ALA A | 79156.501 | -1.048 | 2.341 | 1.00 | 0.00 H |
| ATOM | 1133 | 3НВ | ALA A | 79156.152 | -1.425 | 4.029 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.345 | -2.174 | 0.658 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.058 | -2.154 | -0.771 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.216 | -0.937 | -1.140 | 1.00 | 0.00 C |
| ATOM | 1137 | О | LEU A | 80151.022 | -0.882 | -0.847 | 1.00 | 0.00 O |
| ATOM | 1138 | CB | LEU A | 80152.330 | -3.434 | -1.184 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80151.917 | -3.501 | -2.655 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.133 | -3.730 | -3.540 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80150.885 | -4.597 | -2.871 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.600 | -2.151 | 1.295 | 1.00 | 0.00 H |
| ATOM | 1143 | НА | LEU A | 80153.998 | -2.100 | -1.298 | 1.00 | 0.00 H |
| ATOM | 1144 | 1HB | LEU A | 80152.976 | -4.275 | -0.975 | 1.00 | 0.00 H |
| ATOM | 1145 | 2HB | LEU A | 80151.439 | -3.528 | -0.580 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.471 | -2.559 | -2.939 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | ĽEU A | 80153.887 | -4.268 | -2.984 | 1.00 | 0.00 H |
| ATOM | 1148 | 2HD1 | LEU A | 80153.531 | -2.777 | -3.858 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80152.845 | -4.307 | -4.407 | 1.00 | 0.00 H |
| ATOM | 1150 | 1HD2 | LEU A | 80149.893 | -4.181 | -2.770 | 1.00 | 0.00 H |
| ATOM | 1151 | 2HD2 | LEU A | 80151.027 | -5.374 | -2.134 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80151.002 | -5.012 | -3.860 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.848 | 0.039 | -1.786 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.157 | 1.256 | -2.195 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.307 | 1.009 | -3.437 | 1.00 | 0.00 C |

| ATOM | 1156 | Ο | PHE A | 81151.705 | 0.267 | - 4.335 | 1.00 | 0.00 O |
|------|--------|-----|-------|-----------|--------|---------|------|--------|
| ATOM | 1157 | CB | PHE A | 81153.167 | 2.373 | -2.469 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.932 | 2.803 | -1.249 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81153.577 | 3.955 | -0.564 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81155.004 | 2.057 | -0.788 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81154.278 | 4.354 | 0.558 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81155.708 | 2.451 | 0.334 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81155.345 | 3.600 | 1.008 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.800 | -0.062 | -1.991 | 1.00 | 0.00 H |
| ATOM | 1165 | НА | PHE A | 81151.511 | 1.559 | -1.385 | 1.00 | 0.00 H |
| ATOM | 1166 1 | НВ | PHE A | 81153.881 | 2.030 | -3.203 | 1.00 | 0.00 H |
| ATOM | 1167 2 | 2HB | PHE A | 81152.644 | 3.235 | -2.856 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81152.742 | 4.544 | -0.915 | 1.00 | 0.00 H |
| ATOM | 1169 . | HD2 | PHE A | 81155.289 | 1.158 | -1.315 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81153.992 | 5.253 | 1.082 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81156.543 | 1.860 | 0.683 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.895 | 3.910 | 1.884 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.136 | 1.635 | -3.480 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VALA | 82149.229 | 1.481 | -4.612 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VAL A | 82148.290 | 2.677 | -4.731 | 1.00 | 0.00 C |
| ATOM | 1176 | O | VAL A | 82148.185 | 3.490 | -3.813 | 1.00 | 0.00 O |
| ATOM | 1177 | CB | VAL A | 82148.392 | 0.195 | -4.492 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VAL A | 82149.267 | -1.034 | -4.677 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VAL A | 82147.673 | 0.150 | -3.151 | 1.00 | 0.00 C |
| ATOM | 1180 | Н | VAL A | 82149.874 | 2.213 | -2.734 | 1.00 | 0.00 H |
| ATOM | 1181 | НА | VAL A | 82149.826 | 1.414 | -5.510 | 1.00 | 0.00 H |
| ATOM | 1182 | НВ | VAL A | 82147.648 | 0.200 | -5.274 | 1.00 | 0.00 H |

| ATOM | 1183 1HG1 | VAL A | 82149.980 | -1.095 | -3.866 | 1.00 | 0.00 H |
|------|-----------|---------|-----------|---------|---------|------|--------|
| ATOM | 1184 2HG1 | VAL A | 82149.796 | -0.961 | -5.616 | 1.00 | 0.00 H |
| ATOM | 1185 3HG1 | VALA | 82148.650 | -1.920 | -4.680 | 1.00 | 0.00 H |
| ATOM | 1186 1HG2 | 2 VAL A | 82146.739 | -0.382 | -3.261 | 1.00 | 0.00 H |
| ATOM | 1187 2HG2 | VAL A | 82147.476 | 1.157 | -2.815 | 1.00 | 0.00 H |
| ATOM | 1188 3HG2 | VAL A | 82148.293 | -0.357 | -2.428 | 1.00 | 0.00 H |
| ATOM | 1189 N | LYS A | 83147.610 | 2.775 | -5.868 | 1.00 | 0.00 N |
| ATOM | 1190 CA | LYS A | 83146.677 | 3.871 | -6.108 | 1.00 | 0.00 C |
| ATOM | 1191 C | LYS A | 83145.454 | 3.754 | -5.206 | 1.00 | 0.00 C |
| ATOM | 1192 O | LYS A | 83144.760 | 2.738 | -5.212 | 1.00 | 0.00 O |
| ATOM | 1193 CB | LYS A | 83146.244 | 3.888 | -7.574 | 1.00 | 0.00 C |
| ATOM | 1194 CG | LYS A | 83147.383 | 4.164 | -8.542 | 1.00 | 0.00 C |
| ATOM | 1195 CD | LYS A | 83147.037 | 3.716 | -9.953 | 1.00 | 0.00 C |
| ATOM | 1196 CE | LYS A | 83147.527 | 4.712 | -10.991 | 1.00 | 0.00 C |
| ATOM | 1197 NZ | LYS A | 83147.970 | 4.039 | -12.243 | 1.00 | 0.00 N |
| ATOM | 1198 H | LYS A | 83147.736 | 2.095 | -6.562 | 1.00 | 0.00 H |
| ATOM | 1199 HA | LYS A | 83147.188 | 4.796 | -5.882 | 1.00 | 0.00 H |
| ATOM | 1200 1HB | LYS A | 83145.815 | 2.929 | -7.822 | 1.00 | 0.00 H |
| ATOM | 1201 2HB | LYS A | 83145.494 | 4.653 | -7.708 | 1.00 | 0.00 H |
| ATOM | 1202 1HG | LYS A | 83147.585 | 5.225 | -8.552 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.262 | 3.631 | -8.210 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83147.501 | 2.760 | -10.141 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83145.964 | 3.620 | -10.037 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83146.723 | 5.394 | -11.225 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83148.356 | 5.266 | 10.576 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83147.466 | 3.137 | -12.361 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83148.992 | 3.849 - | -12.204 | 1.00 | 0.00 H |

| ATOM | 1210 | 3HZ | LYS A | 83147.773 | 4.646 - | 13.064 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 1211 | N | LEU A | 84145.197 | 4.803 | -4.432 | 1.00 | 0.00 N |
| ATOM | 1212 | CA | LEU A | 84144.059 | 4.823 | -3.523 | 1.00 | 0.00 C |
| ATOM | 1213 | C | LEU A | 84142.750 | 4.654 | -4.288 | 1.00 | 0.00 C |
| ATOM | 1214 | О | LEU A | 84141.796 | 4.062 | -3.782 | 1.00 | 0.00 O |
| ATOM | 1215 | СВ | LEU A | 84144.039 | 6.133 | -2.733 | 1.00 | 0.00 C |
| ATOM | 1216 | CG | LEU A | 84142.825 | 6.326 | -1.822 | 1.00 | 0.00 C |
| ATOM | 1217 | CD1 | LEU A | 84142.924 | 5.419 | -0.605 | 1.00 | 0.00 C |
| ATOM | 1218 | CD2 | LEU A | 84142.705 | 7.781 | -1.396 | 1.00 | 0.00 C |
| ATOM | 1219 | Н | LEU A | 84145.789 | 5.582 | -4.474 | 1.00 | 0.00 H |
| ATOM | 1220 | НА | LEU A | 84144.169 | 3.999 | -2.834 | 1.00 | 0.00 H |
| ATOM | 1221 | 1HB | LEU A | 84144.931 | 6.175 | -2.125 | 1.00 | 0.00 H |
| ATOM | 1222 | 2HB | LEU A | 84144.066 | 6.952 | -3.437 | 1.00 | 0.00 H |
| ATOM | 1223 | HG | LEU A | 84141.930 | 6.059 | -2.365 | 1.00 | 0.00 H |
| ATOM | 1224 | 1HD1 | LEU A | 84141.946 | 5.308 | -0.159 | 1.00 | 0.00 H |
| ATOM | 1225 | 2HD1 | LEU A | 84143.600 | 5.855 | 0.115 | 1.00 | 0.00 H |
| ATOM | -1226 | 3HD1 | LEU A | 84143.294 | 4.450 | -0.906 | 1.00 | 0.00 H |
| ATOM | 1227 | 1HD2 | LEU A | 84143.646 | 8.115 | -0.986 | 1.00 | 0.00 H |
| ATOM | 1228 | 2HD2 | LEU A | 84141.931 | 7.874 | -0.648 | 1.00 | 0.00 H |
| ATOM | 1229 | 3HD2 | LEU A | 84142.451 | 8.386 | -2.254 | 1.00 | 0.00 H |
| ATOM | 1230 | N | LYS A | 85142.712 | 5.177 | -5.508 | 1.00 | 0.00 N |
| ATOM | 1231 | CA | LYS A | 85141.521 | 5.083 | -6.343 | 1.00 | 0.00 C |
| ATOM | 1232 | C | LYS A | 85141.210 | 3.630 | -6.689 | 1.00 | 0.00 C |
| ATOM | 1233 | О | LYS A | 85140.057 | 3.274 | -6.936 | 1.00 | 0.00 O |
| ATOM | 1234 | CB | LYS A | 85141.707 | 5.896 | -7.627 | 1.00 | 0.00 C |
| ATOM | 1235 | CG | LYS A | 85143.008 | 5.597 | -8.352 | 1.00 | 0.00 C |
| ATOM | 1236 | CD | LYS A | 85142.945 | 6.026 | -9.810 | 1.00 | 0.00 C |

| ATOM | 1237 CE | LYS A | 85142.666 | 4.847 - | 10.728 | 1.00 | 0.00 C |
|------|----------|-------|-----------|---------|---------|------|--------|
| ATOM | 1238 NZ | LYS A | 85143.868 | 4.463 | -11.521 | 1.00 | 0.00 N |
| ATOM | 1239 H | LYS A | 85143.505 | 5.637 | -5.856 | 1.00 | 0.00 H |
| ATOM | 1240 HA | LYS A | 85140.693 | 5.494 | -5.786 | 1.00 | 0.00 H |
| ATOM | 1241 1HB | LYS A | 85140.888 | 5.681 | -8.297 | 1.00 | 0.00 H |
| ATOM | 1242 2HB | LYS A | 85141.691 | 6.947 | -7.379 | 1.00 | 0.00 H |
| ATOM | 1243 1HG | LYS A | 85143.811 | 6.131 | -7.866 | 1.00 | 0.00 H |
| ATOM | 1244 2HG | LYS A | 85143.200 | 4.535 | -8.307 | 1.00 | 0.00 H |
| ATOM | 1245 1HD | LYS A | 85142.156 | 6.754 | -9.927 | 1.00 | 0.00 H |
| ATOM | 1246 2HD | LYS A | 85143.890 | 6.470 - | 10.086 | 1.00 | 0.00 H |
| ATOM | 1247 1HE | LYS A | 85142.358 | 4.003 - | 10.129 | 1.00 | 0.00 H |
| ATOM | 1248 2HE | LYS A | 85141.869 | 5.116 - | 11.406 | 1.00 | 0.00 H |
| ATOM | 1249 1HZ | LYS A | 85143.929 | 3.427 - | 11.599 | 1.00 | 0.00 H |
| ATOM | 1250 2HZ | LYS A | 85144.729 | 4.815 - | 11.058 | 1.00 | 0.00 H |
| ATOM | 1251 3HZ | LYS A | 85143.810 | 4.869 - | 12.477 | 1.00 | 0.00 H |
| ATOM | 1252 N | SER A | 86142.243 | 2.794 | -6.705 | 1.00 | 0.00 N |
| ATOM | 1253 CA | SER A | 86142.077 | 1.380 | -7.019 | 1.00 | 0.00 C |
| ATOM | 1254 C | SER A | 86142.051 | 0.539 | -5.747 | 1.00 | 0.00 C |
| ATOM | 1255 O | SER A | 86142.486 | -0.613 | -5.743 | 1.00 | 0.00 O |
| ATOM | 1256 CB | SER A | 86143.205 | 0.904 | -7.936 | 1.00 | 0.00 C |
| ATOM | 1257 OG | SER A | 86143.371 | 1.779 | -9.038 | 1.00 | 0.00 O |
| ATOM | 1258 H | SER A | 86143.139 | 3.136 | -6.500 | 1.00 | 0.00 H |
| ATOM | 1259 HA | SER A | 86141.134 | 1.264 | -7.533 | 1.00 | 0.00 H |
| ATOM | 1260 1HB | SER A | 86144.128 | 0.869 | -7.378 | 1.00 | 0.00 H |
| ATOM | 1261 2HB | SER A | 86142.972 | -0.083 | -8.308 | 1.00 | 0.00 H |
| ATOM | 1262 HG | SER A | 86142.512 | 1.998 | -9.406 | 1.00 | 0.00 H |
| ATOM | 1263 N | CYS A | 87141.537 | 1.122 | -4.669 | 1.00 | 0.00 N |

| ATOM | 1264 | CA | CYS A | 87141.454 | 0.427 | -3.390 | 1.00 | 0.00 C |
|------|--------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1265 | C | CYS A | 87140.001 | 0.231 | -2.970 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYS A | 87139.186 | 1.148 | -3.073 | 1.00 | 0.00 O |
| ATOM | 1267 | CB | CYS A | 87142.207 | 1.208 | -2.311 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYS A | 87144.005 | 1.180 | -2.501 | 1.00 | 0.00 S |
| ATOM | 1269 | H · | CYS A | 87141.206 | 2.042 | -4.735 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87141.916 | -0.542 | -3.508 | 1.00 | 0.00 H |
| ATOM | 1271 | IНВ | CYS A | 87141.891 | 2.239 | -2.337 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.972 | 0.788 | -1.344 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.394 | 1.095 | -1.627 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.683 | -0.971 | -2.498 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.328 | -1.288 | -2.063 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.292 | -1.575 | -0.563 | 1.00 | 0.00 C |
| ATOM | 1277 | O | ARG A | 88139.234 | -2.142 | -0.010 | 1.00 | 0.00 O |
| ATOM | 1278 | CB · | ARG A | 88137.790 | -2.492 | -2.839 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88136.954 | -2.109 | -4.051 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.509 | -2.558 | -3.902 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.240 | -3.791 | -4.638 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88134.146 | -4.531 | -4.470 | 1.00 | 0.00 C |
| ATOM | 1283 | NH1 | ARG A | 88133.219 | -4.168 | -3.594 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88133.980 | -5.638 | - 5.181 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.377 | -1.660 | -2.441 | 1.00 | 0.00 H |
| ATOM | 1286 | НА | ARG A | 88137.706 | -0.430 | -2.269 | 1.00 | 0.00 H |
| ATOM | 1287 1 | HB | ARG A | 88138.623 | -3.088 | -3.178 | 1.00 | 0.00 H |
| ATOM | 1288 2 | 2HB | ARG A | 88137.176 | - 3.087 | -2.178 | 1.00 | 0.00 H |
| ATOM | 1289 1 | HG | ARG A | 88136.976 | -1.035 | -4.167 | 1.00 | 0.00 H |
| ATOM | 1290 2 | 2HG | ARG A | 88137.378 | -2.575 | -4.929 | 1.00 | 0.00 H |

| ATOM | 1291 | 1HD | ARG A | 88135.304 | -2.724 | -2.854 | 1.00 | 0.00 H |
|--------|--------|--------------|-------|-----------|--------|--------|------|--------|
| ATOM | 1292 | 2HD | ARG A | 88134.862 | -1.778 | -4.275 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88135.910 | -4.082 | -5.292 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88133.338 | -3.334 | -3.054 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88132.399 | -4.728 | -3.472 | 1.00 | 0.00 H |
| ATOM | 1296 | 1 <u>HH2</u> | ARG A | 88134.676 | -5.917 | -5.843 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88133.159 | -6.194 | -5.055 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.198 | -1.187 | 0.118 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89137.048 | -1.408 | 1.560 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.285 | -2.863 | 1.950 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.808 | -3.781 | 1.282 | 1.00 | 0.00 O |
| ATOM | 1302 | CB | PRO A | 89135.594 | -1.013 | 1.832 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.252 | -0.054 | 0.744 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89136.026 | -0.505 | -0.463 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.710 | -0.771 | 2.128 | 1.00 | 0.00 H |
| ATOM | 1306 | 1HB | PRO A | 89134.967 | -1.892 | 1.797 | 1.00 | 0.00 H |
| ATOM | 1307 | 2HB | PRO A | 89135.520 | -0.549 | 2.803 | 1.00 | 0.00 H |
| ATOM | 1308 | 1HG | PRO A | 89134.191 | -0.090 | 0.545 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89135.548 | 0.945 | 1.028 | 1.00 | 0.00 H |
| ATOM | 1310 | 1HD | PRO A | 89135.436 | -1.189 | -1.056 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89136.329 | 0.346 | -1.055 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASPA | 90138.026 | -3.066 | 3.035 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASP A | 90138.326 | -4.409 | 3.514 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.405 | -4.795 | 4.667 | 1.00 | 0.00 C |
| ATOM . | 1315 | O | ASPA | 90137.387 | -4.137 | 5.706 | 1.00 | 0.00 O |
| ATOM | 1316 | CB | ASPA | 90139.786 | -4.499 | 3.961 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASP A | 90140.288 | -5.929 | 4.013 | 1.00 | 0.00 C |

| ATOM | 1318 | OD1 | ASPA | 90139.463 | -6.840 | 4.238 | 1.00 | 0.00 O |
|-------|--------|-----|-------|-----------|---------|-------|------|--------|
| ATOM | 1319 | OD2 | ASPA | 90141.506 | -6.138 | 3.828 | 1.00 | 0.00 O |
| ATOM | 1320 | H | ASPA | 90138.378 | -2.294 | 3.525 | 1.00 | 0.00 H |
| ATOM | 1321 | НА | ASPA | 90138.167 | -5.097 | 2.696 | 1.00 | 0.00 H |
| ATOM | 1322 | lНВ | ASPA | 90140.403 | -3.947 | 3.268 | 1.00 | 0.00 H |
| ATOM | 1323 2 | 2НВ | ASPA | 90139.881 | -4.067 | 4.946 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.640 | -5.865 | 4.475 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91135.716 | -6.338 | 5.498 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91136.321 | -7.495 | 6.286 | 1.00 | 0.00 C |
| ATOM | 1327 | O | SER A | 91135.606 | -8.375 | 6.764 | 1.00 | 0.00 O |
| ATOM | 1328 | CB | SER A | 91134.396 | -6.776 | 4.860 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91133.310 | -6.584 | 5.749 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91136.699 | -6.348 | 3.624 | 1.00 | 0.00 H |
| ATOM | 1331 | НА | SER A | 91135.523 | -5.519 | 6.175 | 1.00 | 0.00 H |
| ATOM | 1332 | IНВ | SER A | 91134.221 | -6.196 | 3.966 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91134.454 | -7.824 | 4.603 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91133.107 | -7.412 | 6.191 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92137.643 | -7.487 | 6.418 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92138.345 | -8.536 | 7.149 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92137.999 | -8.490 | 8.633 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92137.991 | -9.519 | 9.310 | 1.00 | 0.00 O |
| ATOM | 1339 | CB | ARG A | 92139.856 | -8.395 | 6.960 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92140.387 | -9.117 | 5.733 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92140.922 | -10.495 | 6.085 | 1.00 | 0.00 C |
| ATOM. | 1342 | NE | ARG A | 92139.849 | -11.470 | 6.267 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92140.030 | -12.682 | 6.784 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92141.238 | -13.075 | 7.169 | 1.00 | 0.00 N |

| ATOM | 1345 | NH2 | ARG A | 92138.999 | -13.508 | 6.915 | 1.00 | 0.00 N |
|------|--------|-------|-------|-------------|---------|--------|------|--------|
| ATOM | 1346 | Н | ARG A | 92138.160 | -6.758 | 6.014 | 1.00 | 0.00 H |
| ATOM | 1347 | НА | ARG A | 92138.029 | -9.488 | 6.747 | 1.00 | 0.00 H |
| ATOM | 1348 1 | НВ | ARG A | 92140.099 | -7.347 | 6.869 | 1.00 | 0.00 H |
| ATOM | 1349 2 | 2HB | ARG A | 92140.355 | -8.796 | 7.831 | 1.00 | 0.00 H |
| ATOM | 1350 1 | HG | ARG A | 92139.586 | -9.225 | 5.016 | 1.00 | 0.00 H |
| ATOM | 1351 2 | 2HG | ARG A | 92141.183 | -8.530 | 5.299 | 1.00 | 0.00 H |
| ATOM | 1352 1 | HD | ARG A | 92141.568 | -10.830 | 5.287 | 1.00 | 0.00 H |
| ATOM | 1353 2 | 2HD | ARG A | 92141.491 | -10.423 | 7.001 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92138.947 | -11.206 | 5.990 | 1.00 | 0.00 H |
| ATOM | 1355 1 | HH1. | ARG A | 92142.019 - | 12.458 | 7.074 | 1.00 | 0.00 H |
| ATOM | 1356 2 | 2HH1. | ARG A | 92141.367 - | 13.988 | 7.557 | 1.00 | 0.00 H |
| ATOM | 1357 1 | HH2 | ARG A | 92138.087 - | 13.217 | 6.626 | 1.00 | 0.00 H |
| ATOM | 1358 2 | HH2 | ARG A | 92139.135 - | 14.418 | 7.303 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93137.713 | -7.293 | 9.133 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93137.366 | -7.114 | 10.538 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93136.006 | -6.439 | 10.683 | 1.00 | 0.00 C |
| ATOM | 1362 | O | PHE A | 93135.761 | -5.713 | 11.646 | 1.00 | 0.00 O |
| ATOM | 1363 | СВ | PHE A | 93138.437 | -6.284 | 11.248 | 1.00 | 0.00 C |
| ATOM | 1364 | CG | PHE A | 93139.732 | -7.019 | 11.447 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93140.508 | -7.389 | 10.360 | 1.00 | 0.00 C |
| ATOM | 1366 | CD2 | PHE A | 93140.173 | -7.340 | 12.721 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93141.701 | -8.064 | 10.540 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93141.365 | -8.015 | 12.907 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ | PHE A | 93142.129 | -8.378 | 11.815 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93137.736 | -6.511 | 8.543 | 1.00 | 0.00 H |
| ATOM | 1371 | HA | PHE A | 93137.320 | -8.091 | 10.995 | 1.00 | 0.00 H |

| ATOM | 1372 1 | HB | PHE A | 93138.644 | -5.400 | 10.663 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1373 2 | HB | PHE A | 93138.069 | -5.989 | 12.219 | 1.00 | 0.00 H |
| ATOM | 1374 | HD1 | PHE A | 93140.174 | -7.143 | 9.362 | 1.00 | 0.00 H |
| ATOM | 1375 | HD2 | PHE A | 93139.576 | -7.057 | 13.575 | 1.00 | 0.00 H |
| ATOM | 1376 | HE1 | PHE A | 93142.296 | -8.347 | 9.684 | 1.00 | 0.00 H |
| ATOM | 1377 | HE2 | PHE A | 93141.697 | -8.260 | 13.905 | 1.00 | 0.00 H |
| ATOM | 1378 | HZ | PHE A | 93143.060 | -8.906 | 11.957 | 1.00 | 0.00 H |
| ATOM | 1379 | N | ALAA | 94135.123 | -6.684 | 9.719 | 1.00 | 0.00 N |
| ATOM | 1380 | CA | ALAA | 94133.788 | -6.099 | 9.741 | 1.00 | 0.00 C |
| ATOM | 1381 | C | ALA A | 94132.772 | -7.072 | 10.327 | 1.00 | 0.00 C |
| ATOM | 1382 | O | ALA A | 94132.691 | -8.228 | 9.909 | 1.00 | 0.00 O |
| ATOM | 1383 | СВ | ALAA | 94133.373 | -5.682 | 8.337 | 1.00 | 0.00 C |
| ATOM | 1384 | Н | ALA A | 94135.376 | -7.271 | 8.976 | 1.00 | 0.00 H |
| ATOM | 1385 | НА | ALA A | 94133.822 | -5.214 | 10.358 | 1.00 | 0.00 H |
| ATOM | 1386 1 | HB | ALA A | 94134.251 | -5.568 | 7.721 | 1.00 | 0.00 H |
| ATOM | 1387 2 | HB | ALA A | 94132.841 | -4.743 | 8.384 | 1.00 | 0.00 H |
| ATOM | 1388 3 | HB | ALA A | 94132.730 | -6.439 | 7.913 | 1.00 | 0.00 H |
| ATOM | 1389 | N | SER A | 95131.999 | -6.600 | 11.299 | 1.00 | 0.00 N |
| ATOM | 1390 | CA | SER A | 95130.987 | -7.428 | 11.944 | 1.00 | 0.00 C |
| ATOM | 1391 | C | SER A | 95129.662 | -7.353 | 11.194 | 1.00 | 0.00 C |
| ATOM | 1392 | O | SER A | 95129.017 | -6.305 | 11.158 | 1.00 | 0.00 O |
| ATOM | 1393 | CB | SER A | 95130.791 | -6.992 | 13.397 | 1.00 | 0.00 C |
| ATOM | 1394 | OG | SER A | 95130.890 | -5.584 | 13.525 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95132.110 | -5.670 | 11.589 | 1.00 | 0.00 H |
| ATOM | 1396 | НА | SER A | 95131.338 | -8.450 | 11.928 | 1.00 | 0.00 H |
| ATOM | 1397 1 | НВ | SER A | 95129.814 | -7.304 | 13.735 | 1.00 | 0.00 H |
| ATOM | 1398 2 | HB | SER A | 95131.549 | -7.453 | 14.013 | 1.00 | 0.00 H |

| ATOM | 1399 | HG | SER A | 95130.226 | -5.272 | 14.144 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 1400 | N | LEU A | 96129.260 | -8.471 | 10.598 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96128.010 | -8.531 | 9.849 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96127.168 | -9.724 | 10.295 | 1.00 | 0.00 C |
| ATOM | 1403 | Ο | LEU A | 96126.898 | -10.636 | 9.512 | 1.00 | 0.00 O |
| ATOM | 1404 | СВ | LEU A | 96128.294 | -8.620 | 8.348 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96128.449 | -7.275 | 7.638 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96129.872 | -6.756 | 7.782 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEUA | 96128.074 | -7.403 | 6.170 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96129.818 | -9.273 | 10.663 | 1.00 | 0.00 H |
| ATOM | 1409 | HA | LEU A | 96127.459 | -7.624 | 10.049 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96129.204 | -9.186 | 8.209 | 1.00 | 0.00 H |
| ATOM | 1411 | 2HB | LEU A | 96127.483 | -9.158 | 7.881 | 1.00 | 0.00 H |
| ATOM | 1412 | HG | LEU A | 96127.785 | -6.556 | 8.093 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96130.148 | -6.210 | 6.893 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96130.546 | -7.589 | 7.917 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96129.932 | -6.102 | 8.639 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96128.564 | - 6.626 | 5.603 | 1.00 | 0.00 H |
| ATOM | 1417 | 2HD2 | LEU A | 96127.003 | -7.305 | 6.063 | 1.00 | 0.00 H |
| ATOM | 1418 | 3HD2 | LEU A | 96128.385 | -8.368 | 5.800 | 1.00 | 0.00 H |
| ATOM | 1419 | N | GLN A | 97126.757 | -9.711 | 11.559 | 1.00 | 0.00 N |
| ATOM | 1420 | CA | GLN A | 97125.947 | -10.790 | 12.110 | 1.00 | 0.00 C |
| ATOM | 1421 | C | GLN A | 97124.516 | -10.728 | 11.576 | 1.00 | 0.00 C |
| ATOM | 1422 | Ο | GLN A | 97124.045 | -11.665 | 10.932 | 1.00 | 0.00 O |
| ATOM | 1423 | CB | GLN A | 97125.941 | -10.721 | 13.640 | 1.00 | 0.00 C |
| ATOM | 1424 | CG | GLN A | 97126.526 | -11.955 | 14.306 | 1.00 | 0.00 C |
| ATOM | 1425 | CD | GLN A | 97127.328 | -11.623 | 15.549 | 1.00 | 0.00 C |

ATOM OE1 GLN A 97128.215 -10.768 15.519 1.00 0.00 O 1426 **ATOM** NE2 GLN A 97127.020 -12.297 1.00 1427 16.650 0.00 N **ATOM** 97127.004 -8.958 12.134 1.00 1428 Η GLN A 0.00 H **ATOM** HA GLN A 97126.390 -11.726 11.804 1.00 0.00 H1429 **ATOM** 1430 1HB GLN A 97126.519 -9.863 13.952 1.00 0.00 H1431 2HB 13.982 1.00 0.00 H,ATOM GLN A 97124.924 -10.602 97125.719 -12.616 1.00 0.00 H **ATOM** 1432 1HG GLN A 14.585 **ATOM** 1433 2HG GLN A 97127.173 -12.457 13.601 1.00 0.00 H 0.00 H **ATOM** 1434 1HE2 GLN A 97126.303 -12.963 16.600 1.00 **ATOM** 1435 2HE2 GLN A 97127.523 -12.101 17.468 1.00 0.00 H 11.839 **ATOM** 1436 N PRO A 98123.805 -9.618 1.00 0.00 N **ATOM** PRO A 98122.423 -9.441 11.383 1.00 0.00 C 1437 CA **ATOM** 1438 C PRO A 98122.336 -9.185 9.882 1.00 0.00 C 9.190 **ATOM** 1439 О PRO A 98121.504 -9.772 1.00 0.00 O **ATOM** 1440 PRO A 98121.948 -8.215 12.163 1.00 0.00 C CB**ATOM** 1441 CG PRO A 98123.189 -7.437 12.434 1.00 0.00 C 98124.289 -8.450 12.603 **ATOM** 1442 CD PRO A 1.00 0.00 C **ATOM** 1443 HA PROA 98121.811 -10.293 11.637 1.00 0.00 H-7.650 0.00 H**ATOM** 1444 1HB PRO A 98121.251 11.562 1.00 -8.530 13.079 1.00 0.00 H **ATOM** 1445 2HB PRO A 98121.472 **ATOM** 1446 1HG PRO A 98123.404 -6.786 11.600 1.00 0.00 H -6.861 13.341 1.00 0.00 H**ATOM** 1447 2HG PRO A 98123.070 **ATOM** 1448 1HD PRO A 98125.213 -8.076 12.188 1.00 0.00 H**ATOM** 1449 2HD PRO A 98124.416 -8.700 13.646 1.00 0.00 H1.00 0.00 N 99123.200 -8.306 9.385 **ATOM** 1450 N SER A 99123.219 -7.974 7.965 1.00 0.00 C **ATOM** 1451 CA SER A 0.00 C 1452 C 99121.874 7.521 1.00 **ATOM** SER A -7.407

| ATOM | 1453 | О | SER A | 99121.020 | -7.091 | 8.348 | 1.00 | 0.00 O |
|------|--------|-----|---------|------------|--------|-------|------|--------|
| ATOM | 1454 | СВ | SER A | 99123.566 | -9.211 | 7.134 | 1.00 | 0.00 C |
| ATOM | 1455 | OG | SER A | 99124.331 | -8.862 | 5.994 | 1.00 | 0.00 O |
| ATOM | 1456 | Н | SER A | 99123.840 | -7.871 | 9.986 | 1.00 | 0.00 H |
| ATOM | 1457 | НА | SER A | 99123.981 | -7.223 | 7.811 | 1.00 | 0.00 H |
| ATOM | 1458 | НВ | SER A | 99124.136 | -9.899 | 7.738 | 1.00 | 0.00 H |
| ATOM | 1459 2 | 2HB | SER A | 99122.654 | -9.689 | 6.808 | 1.00 | 0.00 H |
| ATOM | 1460 | HG | SER A | 99124.982 | -9.547 | 5.823 | 1.00 | 0.00 H |
| ATOM | 1461 | N | GLY A | 00121.693 | -7.282 | 6.210 | 1.00 | 0.00 N |
| ATOM | 1462 | CA | GLY A | 100120.450 | -6.753 | 5.680 | 1.00 | 0.00 C |
| ATOM | 1463 | C | GLY A 1 | 00119.356 | -7.803 | 5.611 | 1.00 | 0.00 C |
| ATOM | 1464 | О | GLY A | 00119.639 | -8.982 | 5.399 | 1.00 | 0.00 O |
| ATOM | 1465 | Н | GLY A 1 | 00122.411 | -7.550 | 5.597 | 1.00 | 0.00 H |
| ATOM | 1466 | HA | GLY A 1 | 00120.118 | -5.944 | 6.312 | 1.00 | 0.00 H |
| ATOM | 1467 2 | 2HA | GLY A 1 | 00120.628 | -6.370 | 4.686 | 1.00 | 0.00 H |
| ATOM | 1468 | N | PRO A | 101118.085 | -7.404 | 5.789 | 1.00 | 0.00 N |
| ATOM | 1469 | CA | PRO A | 101116.952 | -8.333 | 5.743 | 1.00 | 0.00 C |
| ATOM | 1470 | C | PRO A 1 | 01116.660 | -8.821 | 4.328 | 1.00 | 0.00 C |
| ATOM | 1471 | О | PRO A | 101116.427 | -8.023 | 3.421 | 1.00 | 0.00 O |
| ATOM | 1472 | CB | PRO A | 101115.786 | -7.494 | 6.269 | 1.00 | 0.00 C |
| ATOM | 1473 | CG | PRO A | 101116.154 | -6.088 | 5.942 | 1.00 | 0.00 C |
| ATOM | 1474 | CD | PRO A | 101117.653 | -6.016 | 6.049 | 1.00 | 0.00 C |
| ATOM | 1475 | HA | PRO A | 101117.110 | -9.182 | 6.391 | 1.00 | 0.00 H |
| ATOM | 1476 | НВ | PRO A 1 | 01114.873 | -7.791 | 5.773 | 1.00 | 0.00 H |
| ATOM | 1477 2 | 2HB | PRO A 1 | 01115.686 | -7.638 | 7.335 | 1.00 | 0.00 H |
| ATOM | 1478 | IHG | PRO A | 101115.838 | -5.850 | 4.937 | 1.00 | 0.00 H |
| ATOM | 1479 2 | 2HG | PRO A | 101115.696 | -5.414 | 6.650 | 1.00 | 0.00 H |

| ATOM | 1480 1HD | PRO A 101118.052 -5.343 | 5.304 1.00 0.00 H |
|------|----------|--------------------------|-------------------|
| ATOM | 1481 2HD | PRO A 101117.947 -5.701 | 7.039 1.00 0.00 H |
| ATOM | 1482 N | SER A 102116.674 -10.138 | 4.148 1.00 0.00 N |
| ATOM | 1483 CA | SER A 102116.412 -10.733 | 2.842 1.00 0.00 C |
| ATOM | 1484 C | SER A 102116.109 -12.222 | 2.974 1.00 0.00 C |
| ATOM | 1485 O | SER A 102114.991 -12.664 | 2.712 1.00 0.00 O |
| ATOM | 1486 CB | SER A 102117.608 -10.524 | 1.913 1.00 0.00 C |
| ATOM | 1487 OG | SER A 102118.116 -9.206 | 2.023 1.00 0.00 O |
| ATOM | 1488 H | SER A 102116.867 -10.723 | 4.910 1.00 0.00 H |
| ATOM | 1489 HA | SER A 102115.549 -10.239 | 2.421 1.00 0.00 H |
| ATOM | 1490 1HB | SER A 102118.391 -11.220 | 2.174 1.00 0.00 H |
| ATOM | 1491 2HB | SER A 102117.301 -10.695 | 0.891 1.00 0.00 H |
| ATOM | 1492 HG | SER A 102117.394 -8.577 | 1.950 1.00 0.00 H |
| ATOM | 1493 N | SER A 103117.113 -12.991 | 3.383 1.00 0.00 N |
| ATOM | 1494 CA | SER A 103116.954 -14.431 | 3.549 1.00 0.00 C |
| ATOM | 1495 C | SER A 103116.257 -14.753 | 4.867 1.00 0.00 C |
| ATOM | 1496 O | SER A 103115.461 -15.689 | 4.948 1.00 0.00 O |
| ATOM | 1497 CB | SER A 103118.316 -15.125 | 3.496 1.00 0.00 C |
| ATOM | 1498 OG | SER A 103119.347 -14.261 | 3.943 1.00 0.00 O |
| ATOM | 1499 H | SER A 103117.982 -12.580 | 3.576 1.00 0.00 H |
| ATOM | 1500 HA | SER A 103116.344 -14.793 | 2.735 1.00 0.00 H |
| ATOM | 1501 1HB | SER A 103118.297 -15.999 | 4.129 1.00 0.00 H |
| ATOM | 1502 2HB | SER A 103118.528 -15.422 | 2.480 1.00 0.00 H |
| ATOM | 1503 HG | SER A 103119.084 -13.850 | 4.770 1.00 0.00 H |
| ATOM | 1504 N | GLY A 104116.563 -13.971 | 5.898 1.00 0.00 N |
| ATOM | 1505 CA | GLY A 104115.957 -14.190 | 7.198 1.00 0.00 C |
| ATOM | 1506 C | GLY A 104116.797 -13.632 | 8.330 1.00 0.00 C |

ATOM 1507 O GLY A 104116.544 -12.483 8.749 1.00 0.00 O 1508 OXT GLY A 104117.710 -14.346 1.00 0.00 O **ATOM** 8.800 1509 H GLY A 104117.204 -13.241 1.00 0.00 H **ATOM** 5.775 1510 1HA GLY A 104114.988 -13.713 1.00 0.00 H**ATOM** 7.216 **ATOM** 1511 2HA GLY A 104115.828 -15.251 7.349 1.00 0.00 HTER 1512 GLY A 104 **ENDMDL**

Three-Dimensional Structure Coordinate Table 4

1121.720 20.634 -14.920 1.00 0.00 N ATOM 1 N GLY A ATOM 2 CA GLY A 1122.817 20.620 -15.926 1.00 0.00 C ATOM 3 C GLY A 1124.008 19.798 -15.473 1.00 0.00 C ATOM 4 O GLY A 1124.328 18.773 -16.074 1.00 0.00 O ATOM 5 1H GLY A 1121.802 19.811 -14.289 1.00 0.00 H ATOM 6 2H GLY A 1120.797 20.600 -15.398 1.00 0.00 H ATOM 7 3H GLY A 1121.770 21.502 -14.350 1.00 0.00 H ATOM 8 1HA GLY A 1.00 0.00 H 1122.439 20.205 -16.849 ATOM 9 2HA GLY A 1123.140 21.634 -16.106 1.00 0.00 H ATOM10 N SER A 2124.667 20.251 -14.411 1.00 0.00 N ATOM11 CA SER A 2125.830 19.552 -13.878 1.00 0.00 C ATOM12 C SER A 2125.464 18.765 -12.623 1.00 0.00 C 1.00 0.00 O ATOM13 O SER A 2126.259 18.661 -11.690 ATOM14 CB SER A 2126.948 20.547 -13.561 1.00 0.00 C 2126.520 21.513 -12.617 1.00 0.00 O ATOM15 OG SER A 2124.363 21.075 -13.976 1.00 0.00 H ATOM16 H SER A 1.00 0.00 H ATOM17 HA SER A 2126.177 18.862 -14.633 1.00 0.00 H ATOM18 1HB SER A 2127.796 20.015 -13.156

| ATOM19 | 2HB | SER A | 2127.243 | 21.054 -1 | 4.469 | 1.00 | 0.00 H |
|--------|-----|-------|----------|-----------|--------|------|--------|
| ATOM20 | HG | SER A | 2126.598 | 22.391 - | 12.998 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3124.255 | 18.213 - | 12.610 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3123.782 | 17.436 - | 11.469 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3123.253 | 16.078 -1 | 1.920 | 1.00 | 0.00 C |
| ATOM24 | O | SER A | 3123.214 | 15.780 - | 13.113 | 1.00 | 0.00 O |
| ATOM25 | СВ | SER A | 3122.690 | 18.201 - | 10.721 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3122.954 | 19.592 - | 10.713 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3123.666 | 18.332 - | 13.384 | 1.00 | 0.00 H |
| ATOM28 | HA | SER A | 3124.619 | 17.280 - | 10.805 | 1.00 | 0.00 H |
| ATOM29 | 1HB | SER A | 3121.739 | 18.031 -1 | 1.206 | 1.00 | 0.00 H |
| ATOM30 | 2HB | SER A | 3122.641 | 17.848 | -9.701 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3123.781 | 19.758 - | 10.252 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4122.847 | 15.258 - | 10.956 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4122.325 | 13.942 - | 11.272 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4121.131 | 13.570 - | 10.416 | 1.00 | 0.00 C |
| ATOM35 | O | GLY A | 4120.014 | 13.442 - | 10.917 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4122.901 | 15.549 - | 10.021 | 1.00 | 0.00 H |
| ATOM37 | 1HA | GLY A | 4122.029 | 13.925 - | 12.310 | 1.00 | 0.00 H |
| ATOM38 | 2HA | GLY A | 4123.105 | 13.211 - | 11.120 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5121.366 | 13.394 | -9.120 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5120.300 | 13.034 | -8.191 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5120.725 | 13.292 | -6.750 | 1.00 | 0.00 C |
| ATOM42 | О | SER A | 5121.804 | 13.829 | -6.496 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5119.918 | 11.564 | -8.367 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5118.602 | 11.319 | -7.902 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5122.278 | 13.510 | -8.780 | 1.00 | 0.00 H |

| ATOM46 | HA | SER A | 5119.443 | 13.650 | -8.417 | 1.00 | 0.00 H | |
|--------|-----|-------|----------|--------|--------|------|--------|--|
| ATOM47 | 1HB | SER A | 5119.969 | 11.303 | -9.414 | 1.00 | 0.00 H | |
| ATOM48 | 2HB | SER A | 5120.605 | 10.946 | -7.809 | 1.00 | 0.00 H | |
| ATOM49 | HG | SER A | 5117.985 | 11.880 | -8.377 | 1.00 | 0.00 H | |
| ATOM50 | N | SER A | 6119.871 | 12.904 | -5.808 | 1.00 | 0.00 N | |
| ATOM51 | CA | SER A | 6120.158 | 13.094 | -4.391 | 1.00 | 0.00 C | |
| ATOM52 | C | SER A | 6120.904 | 11.891 | -3.822 | 1.00 | 0.00 C | |
| ATOM53 | O | SER A | 6120.766 | 10.772 | -4.314 | 1.00 | 0.00 O | |
| ATOM54 | СВ | SER A | 6118.860 | 13.318 | -3.612 | 1.00 | 0.00 C | |
| ATOM55 | OG | SER A | 6118.541 | 14.697 | -3.538 | 1.00 | 0.00 O | |
| ATOM56 | Н | SER A | 6119.027 | 12.481 | -6.073 | 1.00 | 0.00 H | |
| ATOM57 | HA | SER A | 6120.782 | 13.969 | -4.293 | 1.00 | 0.00 H | |
| ATOM58 | 1HB | SER A | 6118.052 | 12.801 | -4.106 | 1.00 | 0.00 H | |
| ATOM59 | 2HB | SER A | 6118.975 | 12.933 | -2.609 | 1.00 | 0.00 H | |
| ATOM60 | HG | SER A | 6118.107 | 14.880 | -2.702 | 1.00 | 0.00 H | |
| ATOM61 | N | GLY A | 7121.697 | 12.132 | -2.782 | 1.00 | 0.00 N | |
| ATOM62 | CA | GLY A | 7122.455 | 11.059 | -2.163 | 1.00 | 0.00 C | |
| ATOM63 | C | GLY A | 7123.939 | 11.360 | -2.100 | 1.00 | 0.00 C | |
| ATOM64 | O | GLY A | 7124.349 | 12.392 | -1.568 | 1.00 | 0.00 O | |
| ATOM65 | Н | GLY A | 7121.768 | 13.044 | -2.433 | 1.00 | 0.00 H | |
| ATOM66 | 1HA | GLY A | 7122.086 | 10.908 | -1.159 | 1.00 | 0.00 H | |
| ATOM67 | 2HA | GLY A | 7122.306 | 10.153 | -2.730 | 1.00 | 0.00 H | |
| ATOM68 | N | LEU A | 8124.747 | 10.455 | -2.645 | 1.00 | 0.00 N | |
| ATOM69 | CA | LEU A | 8126.195 | 10.628 | -2.648 | 1.00 | 0.00 C | |
| ATOM70 | C | LEU A | 8126.735 | 10.727 | -1.225 | 1.00 | 0.00 C | |
| ATOM71 | O | LEU A | 8126.956 | 11.822 | -0.708 | 1.00 | 0.00 O | |
| ATOM72 | СВ | LEU A | 8126.578 | 11.881 | -3.439 | 1.00 | 0.00 C | |

| ATOM73 | CG | LEU A | 8126.391 | 11.771 | -4.954 | 1.00 | 0.00 C | |
|--------|---------------|-------|-----------|--------|--------|------|--------|--|
| ATOM74 | CD1 | LEU A | 8125.132 | 12.503 | -5.392 | 1.00 | 0.00 C | |
| ATOM75 | CD2 | LEU A | 8127.609 | 12.320 | -5.684 | 1.00 | 0.00 C | |
| ATOM76 | Н | LEU A | 8124.360 | 9.653 | -3.053 | 1.00 | 0.00 H | |
| ATOM77 | HA | LEU A | 8126.631 | 9.764 | -3.127 | 1.00 | 0.00 H | |
| ATOM78 | 1HB | LEU A | 8125.979 | 12.704 | -3.080 | 1.00 | 0.00 H | |
| ATOM79 | 2HB | LEU A | 8127.617 | 12.101 | -3.241 | 1.00 | 0.00 H | |
| ATOM80 | HG | LEU A | 8126.281 | 10.731 | -5.222 | 1.00 | 0.00 H | |
| ATOM81 | 1HD1 | LEU A | 8125.389 | 13.502 | -5.716 | 1.00 | 0.00 H | |
| ATOM82 | 2HD1 | LEU A | 8124.442 | 12.560 | -4.564 | 1.00 | 0.00 H | |
| ATOM83 | 3HD1 | LEU A | 8124.669 | 11.968 | -6.208 | 1.00 | 0.00 H | |
| ATOM84 | 1HD2 | LEU A | 8127.471 | 12.206 | -6.749 | 1.00 | 0.00 H | |
| ATOM85 | 2HD2 | LEU A | 8128.489 | 11.776 | -5.375 | 1.00 | 0.00 H | |
| ATOM86 | 3HD2 | LEU A | 8127.731 | 13.366 | -5.447 | 1.00 | 0.00 H | |
| ATOM87 | N | ALA A | 9126.946 | 9.575 | -0.597 | 1.00 | 0.00 N | |
| ATOM88 | CA | ALA A | 9127.461 | 9.530 | 0.766 | 1.00 | 0.00 C | |
| ATOM89 | C | ALAA | 9128.987 | 9.538 | 0.777 | 1.00 | 0.00 C | |
| ATOM90 | О | ALAA | 9129.620 | 8.618 | 1.295 | 1.00 | 0.00 O | |
| ATOM91 | CB | ALA A | 9126.930 | 8.302 | 1.490 | 1.00 | 0.00 C | |
| ATOM92 | Н | ALA A | 9126.752 | 8.734 | -1.062 | 1.00 | 0.00 H | |
| ATOM93 | HA | ALA A | 9127.103 | 10.408 | 1.285 | 1.00 | 0.00 H | |
| ATOM94 | 1HB | ALA A | 9126.984 | 7.446 | 0.834 | 1.00 | 0.00 H | |
| ATOM95 | 2HB | ALA A | 9125.902 | 8.470 | 1.778 | 1.00 | 0.00 H | |
| ATOM96 | 3HB | ALA A | 9127.525 | 8.119 | 2.372 | 1.00 | 0.00 H | |
| ATOM97 | N | MET A | 10129.571 | 10.584 | 0.201 | 1.00 | 0.00 N | |
| ATOM98 | CA | MET A | 10131.023 | 10.712 | 0.145 | 1.00 | 0.00 C | |
| ATOM99 | $^{\prime}$ C | MET A | 10131.429 | 12.104 | -0.337 | 1.00 | 0.00 C | |

| ATOM | 100 | О | MET A | 10132.025 | 12.252 | -1.405 | 1.00 | 0.00 O | |
|--------|-------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 101 | СВ | MET A | 10131.614 | 9.645 | -0.779 | 1.00 | 0.00 C | |
| ATOM . | 102 | CG | MET A | 10130.848 | 9.478 | -2.083 | 1.00 | 0.00 C | |
| ATOM | 103 | SD | MET A | 10131.914 | 9.566 | -3.535 | 1.00 | 0.00 S | |
| ATOM | 104 | CE | MET A | 10131.189 | 10.954 | -4.404 | 1.00 | 0.00 C | |
| ATOM | 105 | Н | MET A | 10129.013 | 11.286 | -0.194 | 1.00 | 0.00 H | |
| ATOM | 106 | НА | MET A | 10131.407 | 10.564 | 1.143 | 1.00 | 0.00 H | |
| ATOM | 107 1 | НВ | MET A | 10132.633 | 9.913 | -1.014 | 1.00 | 0.00 H | |
| ATOM | 108 2 | 2HB | MET A | 10131.611 | 8.697 | -0.261 | 1.00 | 0.00 H | |
| ATOM | 109 1 | HG | MET A | 10130.356 | 8.517 | -2.075 | 1.00 | 0.00 H | |
| ATOM | 110 2 | HG | MET A | 10130.106 | 10.259 | -2.151 | 1.00 | 0.00 H | |
| ATOM | 111 1 | HE | MET A | 10130.247 | 10.653 | -4.838 | 1.00 | 0.00 H | |
| ATOM | 112 2 | HE | MET A | 10131.859 | 11.279 | -5.186 | 1.00 | 0.00 H | |
| ATOM | 113 3 | HE | MET A | 10131.023 | 11.765 | -3.711 | 1.00 | 0.00 H | |
| ATOM | 114 | N | PRO A | 11131.111 | 13.149 | 0.447 | 1.00 | 0.00 N | |
| ATOM | 115 | CA | PRO A | 11131.448 | 14.531 | 0.093 | 1.00 | 0.00 C | |
| ATOM | 116 | C | PRO A | 11132.950 | 14.732 | -0.102 | 1.00 | 0.00 C | |
| ATOM | 117 | О | PRO A | 11133.376 | 15.329 | -1.090 | 1.00 | 0.00 O | |
| ATOM | 118 | СВ | PRO A | 11130.946 | 15.355 | 1.283 | 1.00 | 0.00 C | |
| ATOM | 119 | CG | PRO A | 11129.966 | 14.479 | 1.987 | 1.00 | 0.00 C | |
| ATOM | 120 | CD | PRO A | 11130.402 | 13.063 | 1.735 | 1.00 | 0.00 C | |
| ATOM | 121 | HA | PRO A | 11130.931 | 14.840 | -0.803 | 1.00 | 0.00 H | |
| ATOM | 122 1 | НВ | PRO A | 11131.778 | 15.610 | 1.923 | 1.00 | 0.00 H | |
| ATOM | 123 2 | ΣНВ | PRO A | 11130.476 | 16.258 | 0.923 | 1.00 | 0.00 H | |
| ATOM | 124 1 | HG | PRO A | 11129.982 | 14.690 | 3.045 | 1.00 | 0.00 H | |
| ATOM | 125 2 | 2HG | PRO A | 11128.975 | 14.641 | 1.587 | 1.00 | 0.00 H | |
| ATOM | 126 | HD | PRO A | 11131.065 | 12.727 | 2.519 | 1.00 | 0.00 H | |

| ATOM | 127 2 | 2HD | PRO A | 11129.544 | 12.412 | 1.659 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 128 | N | PRO A | 12133.779 | 14.235 | 0.835 | 1.00 | 0.00 N |
| ATOM | 129 | CA | PRO A | 12135.238 | 14.369 | 0.742 | 1.00 | 0.00 C |
| ATOM | 130 | C | PRO A | 12135.783 | 13.801 | -0.562 | 1.00 | 0.00 C |
| ATOM | 131 | O | PRO A | 12136.871 | 14.169 | -1.006 | 1.00 | 0.00 O |
| ATOM | 132 | СВ | PRO A | 12135.755 | 13.558 | 1.934 | 1.00 | 0.00 C |
| ATOM | 133 | CG | PRO A | 12134.615 | 13.509 | 2.890 | 1.00 | 0.00 C |
| ATOM | 134 | CD | PRO A | 12133.371 | 13.501 | 2.049 | 1.00 | 0.00 C |
| ATOM | 135 | HA | PRO A | 12135.546 | 15.399 | 0.841 | 1.00 | 0.00 H |
| ATOM | 136 1 | lНВ | PRO A | 12136.037 | 12.568 | 1.604 | 1.00 | 0.00 H |
| ATOM | 137 2 | 2HB | PRO A | 12136.611 | 14.055 | 2.366 | 1.00 | 0.00 H |
| ATOM | 138 1 | IHG | PRO A | 12134.672 | 12.609 | 3.484 | 1.00 | 0.00 H |
| ATOM | 139 2 | 2HG | PRO A | 12134.632 | 14.382 | 3.526 | 1.00 | 0.00 H |
| ATOM | 140 1 | IHD | PRO A | 12133.084 | 12.488 | 1.809 | 1.00 | 0:00 H |
| ATOM | 141 2 | 2HD | PRO A | 12132.570 | 14.012 | 2.558 | 1.00 | 0.00 H |
| ATOM | 142 | N | GLY A | 13135.020 | 12.900 | -1.175 | 1.00 | 0.00 N |
| ATOM | 143 | CA | GLY A | 13135.443 | 12.293 | -2.423 | 1.00 | 0.00 C |
| ATOM | 144 | C | GLY A | 13135.739 | 10.814 | -2.278 | 1.00 | 0.00 C |
| ATOM | 145 | O | GLY A | 13135.196 | 10.149 | -1.395 | 1.00 | 0.00 O |
| ATOM | 146 | Н | GLY A | 13134.162 | 12.644 | -0.774 | 1.00 | 0.00 H |
| ATOM | 147 | 1HA | GLY A | 13134.662 | 12.423 | -3.156 | 1.00 | 0.00 H |
| ATOM | 148 2 | 2HA | GLY A | 13136.335 | 12.795 | -2.771 | 1.00 | 0.00 H |
| ATOM | 149 | N | ASN A | 14136.601 | 10.296 | -3.147 | 1.00 | 0.00 N |
| ATOM | 150 | CA | ASN A | 14136.968 | 8.885 | -3.112 | 1.00 | 0.00 C |
| ATOM | 151 | C | ASN A | 14135.742 | 7.999 | -3.313 | 1.00 | 0.00 C |
| ATOM | 152 | O | ASN A | 14134.635 | 8.494 | -3.530 | 1.00 | 0.00 O |
| ATOM | 153 | СВ | ASN A | 14137.644 | 8.545 | -1.783 | 1.00 | 0.00 C |

| ATOM | 154 | CG | ASN A | 14138.954 | 9.284 | -1.595 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 155 | OD1 | ASN A | 14139.305 | 10.161 | -2.385 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14139.687 | 8.933 | -0.545 | 1.00 | 0.00 N |
| ATOM | 157 | Н | ASN A | 14137.000 | 10.876 | -3.828 | 1.00 | 0.00 H |
| ATOM | 158 | НА | ASN A | 14137.664 | 8.704 | -3.917 | 1.00 | 0.00 H |
| ATOM | 159 | lНВ | ASN A | 14136.983 | 8.810 | -0.971 | 1.00 | 0.00 H |
| ATOM | 160 2 | 2HB | ASN A | 14137.842 | 7.484 | -1.747 | 1.00 | 0.00 H |
| ATOM | 161 | HD2 | ASN A | 14139.345 | 8.227 | 0.043 | 1.00 | 0.00 H |
| ATOM | 162 2 | 2HD2 | ASN A | 14140.538 | 9.395 | -0.399 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15135.948 | 6.689 | -3.242 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15134.858 | 5.734 | -3.416 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15133.890 | 5.791 | -2.239 | 1.00 | 0.00 C |
| ATOM | 166 | O | SER A | 15132.711 | 6.101 | -2.407 | 1.00 | 0.00 O |
| ATOM | 167 | CB | SER A | 15135.414 | 4.317 | -3.566 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15136.208 | 3.959 | -2.448 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15136.852 | 6.355 | -3.068 | 1.00 | 0.00 H |
| ATOM | 170 | НА | SER A | 15134.326 | 5.999 | -4.317 | 1.00 | 0.00 H |
| ATOM | 171 1 | НВ | SER A | 15134.595 | 3.618 | -3.647 | 1.00 | 0.00 H |
| ATOM | 172 2 | 2HB | SER A | 15136.023 | 4.263 | -4.456 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15137.082 | 3.698 | -2.747 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16134.398 | 5.491 | -1.048 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.578 | 5.509 | 0.159 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16134.260 | 6.307 | 1.267 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.836 | 7.413 | 1.599 | 1.00 | 0.00 O |
| ATOM | 178 | CB | HIS A | 16133.304 | 4.080 | 0.634 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16131.900 | 3.624 | 0.378 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16131.007 | 3.335 | 1.388 | 1.00 | 0.00 N |

| ATOM | 181 | CD2 | HIS A | 16131.237 | 3.409 | -0.782 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|-------|--------|------|----------|
| ATOM | 182 | CE1 | HIS A | 16129.855 | 2.961 | 0.860 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16129.968 | 2.997 | -0.455 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16135.345 | 5.253 | -0.978 | 1.00 | 0.00 H |
| ATOM | 185 | НА | HIS A | 16132.640 | 5.984 | -0.086 | 1.00 | 0.00 H |
| ATOM | 186 | HB | HIS A | 16133.970 | 3.403 | 0.122 | 1.00 | 0.00 H |
| ATOM | 187 2 | 2HB | HIS A | 16133.485 | 4.019 | 1.698 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16131.190 | 3.395 | 2.350 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16131.632 | 3.536 | -1.780 | 1.00 | 0.00 H |
| ATOM | 190 | HE1 | HIS A | 16128.971 | 2.675 | 1.411 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16129.289 | 2.685 | -1.088 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.318 | 5.736 | 1.834 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17136.041 | 6.408 | 2.898 | 1.00 | 0.00 C |
| ATOM | 194 | C | GLY A | 17137.368 | 5.742 | 3.205 | 1.00 | 0.00 C |
| ATOM | 195 | O | GLY A | 17137.614 | 5.325 | 4.336 | 1.00 | , 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.609 | 4.853 | 1.527 | 1.00 | 0.00 H |
| ATOM | 197 | IHA | GLY A | 17136.223 | 7.431 | 2.604 | 1.00 | 0.00 H |
| ATOM | 198 2 | 2HA | GLY A | 17135.433 | 6.403 | 3.791 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18138.224 | 5.641 | 2.194 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.533 | 5.020 | 2.360 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.585 | 6.058 | 2.735 | 1.00 | 0.00 C |
| ATOM | 202 | O | LEU A | 18140.997 | 6.868 | 1.904 | 1.00 | 0.00 O |
| ATOM | 203 | СВ | LEU A | 18139.946 | 4.299 | 1.074 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18138.884 | 3.370 | 0.484 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18139.224 | 3.020 | -0.957 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18138.754 | 2.110 | 1.325 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.969 | 5.991 | 1.314 | 1.00 | 0.00 H |

| ATOM | 208 HA LEUA | 18139.458 | 4.296 | 3.158 | 1.00 | 0.00 H |
|--------|----------------|-----------|-------|--------|------|--------|
| ATOM | 209 1HB LEU A | 18140.195 | 5.046 | 0.333 | 1.00 | 0.00 H |
| ATOM | 210 2HB LEU A | 18140.828 | 3.714 | 1.282 | 1.00 | 0.00 H |
| ATOM | 211 HG LEUA | 18137.929 | 3.877 | 0.487 | 1.00 | 0.00 H |
| ATOM | 212 1HD1 LEU A | 18140.293 | 3.082 | -1.099 | 1.00 | 0.00 H |
| ĄŢOM | 213 2HD1 LEU A | 18138.731 | 3.712 | -1.622 | 1.00 | 0.00 H |
| ATOM | 214 3HD1 LEU A | 18138.890 | 2.015 | -1.171 | 1.00 | 0.00 H |
| ATOM | 215 1HD2 LEU A | 18139.718 | 1.634 | 1.411 | 1.00 | 0.00 H |
| ATOM | 216 2HD2 LEU A | 18138.058 | 1.432 | 0.852 | 1.00 | 0.00 H |
| ATOM | 217 3HD2 LEU A | 18138.390 | 2.369 | 2.308 | 1.00 | 0.00 H |
| ATOM | 218 N GLU A | 19141.017 | 6.028 | 3.992 | 1.00 | 0.00 N |
| ATOM | 219 CA GLUA | 19142.022 | 6.965 | 4.478 | 1.00 | 0.00 C |
| ATOM - | 220 C GLUA | 19143.071 | 6.248 | 5.321 | 1.00 | 0.00 C |
| ATOM | 221 O GLUA | 19143.018 | 5.031 | 5.491 | 1.00 | 0.00 O |
| ATOM | 222 CB GLUA | 19141.360 | 8.074 | 5.299 | 1.00 | 0.00 C |
| ATOM | 223 CG GLU A | 19140.503 | 7.556 | 6.441 | 1.00 | 0.00 C |
| ATOM | 224 CD GLUA | 19139.214 | 8.339 | 6.604 | 1.00 | 0.00 C |
| ATOM | 225 OE1 GLU A | 19138.659 | 8.787 | 5.579 | 1.00 | 0.00 O |
| ATOM | 226 OE2 GLU A | 19138.761 | 8.502 | 7.756 | 1.00 | 0.00 O |
| ATOM | 227 H GLU A | 19140.651 | 5.358 | 4.607 | 1.00 | 0.00 H |
| ATOM | 228 HA GLUA | 19142.506 | 7.405 | 3.619 | 1.00 | 0.00 H |
| ATOM | 229 1HB GLU A | 19142.132 | 8.706 | 5.714 | 1.00 | 0.00 H |
| ATOM | 230 2HB GLU A | 19140.735 | 8.664 | 4.646 | 1.00 | 0.00 H |
| ATOM | 231 1HG GLU A | 19140.256 | 6.523 | 6.249 | 1.00 | 0.00 H |
| ATOM | 232 2HG GLU A | 19141.068 | 7.626 | 7.359 | 1.00 | 0.00 H |
| ATOM | 233 N VALA | 20144.023 | 7.011 | 5.846 | 1.00 | 0.00 N |
| ATOM | 234 CA VALA | 20145.085 | 6.447 | 6.672 | 1.00 | 0.00 C |

ATOM 235 C VALA 20144.518 5.816 7.939 1.00 0.00 C **ATOM** VAL A 20143.685 6.411 8.621 1.00 0.00 O 236 O **ATOM** CB VALA 20146.122 7.065 1.00 0.00 C 237 7.518 **ATOM** CG1 VALA 20147.296 6.884 7.795 1.00 0.00 C 238 **ATOM** 239 CG2 VALA 20146.598 8.279 5.835 1.00 0.00 C VAL A 20144.013 7.976 5.675 1.00 0.00 H**ATOM** 240 Η HA VALA 20145.587 5.685 6.095 1.00 0.00 H **ATOM** 241 **ATOM** 242 HB VALA 20145.648 8.220 7.734 1.00 0.00 H **ATOM** 243 1HG1 VAL A 20148.120 7.582 7.825 1.00 0.00 H **ATOM** 244 2HG1 VAL A 20147.602 5.988 7.276 1.00 0.00 H **ATOM** 245 3HG1 VAL A 20147.000 6.632 8.802 1.00 0.00 H **ATOM** 246 1HG2 VAL A 20146.673 9.330 6.069 1.00 0.00 H**ATOM** 247 2HG2 VAL A 20145.893 8.139 5.029 1.00 0.00 H 248 3HG2 VAL A 20147.567 7.907 5.535 1.00 0.00 H **ATOM ATOM** 249 N GLY A 21144.974 4.607 8.247 1.00 0.00 N **ATOM** 250 CA GLY A 21144.501 3.914 9.431 1.00 0.00 C 0.00 C **ATOM** 251 C GLY A 21143.495 2.828 9.106 1.00 **ATOM** 252 Ο GLY A 21143.520 1.751 9.699 1.00 0.00 O **ATOM** 253 H GLY A 21145.639 4.181 7.665 1.00 0.00 H9.935 1.00 **ATOM** 254 1HA GLY A 21145.347 3.468 0.00 H **ATOM** 255 2HA GLY A 21144.040 4.631 10.093 1.00 0.00 H 1.00 **ATOM** 256 N SER A 22142.605 3.114 8.159 0.00 N **ATOM** 257 CA SER A 22141.584 2.153 7.757 1.00 0.00 C **ATOM** 258 C SER A 22142.168 1.099 6.821 1.00 0.00 C SER A 22143.084 6.049 1.00 0.00 O **ATOM** 259 О 1.379 7.070 1.00 0.00 C **ATOM** CB SER A 22140.421 2.872 260 1.00 0.00 O **ATOM** 261 OG SER A 22139.627 3.571 8.012

| ATOM | 262 | Н | SER A | 22142.636 | 3.990 | 7.723 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 263 | HA | SER A | 22141.218 | 1.664 | 8.647 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.810 | 3.578 | 6.352 | 1.00 | 0.00 H |
| ATOM | 265 | 2HB | SER A | 22139.803 | 2.146 | 6.563 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22139.120 | 4.251 | 7.562 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.632 | -0.115 | 6.897 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23142.098 | -1.212 | 6.057 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.431 | -1.171 | 4.687 | 1.00 | 0.00 C |
| ATOM | 270 | О | LEU A | 23140.263 | -0.802 | 4.564 | 1.00 | 0.00 O |
| ATOM | 271 | СВ | LEU A | 23141.820 | -2.555 | 6.734 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23142.685 | -2.855 | 7.958 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23141.930 | -3.730 | 8.945 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.986 | -3.523 | 7.539 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.904 | -0.277 | 7.533 | 1.00 | 0.00 H |
| ATOM | 276 | HA | LEU A | 23143.165 | -1.098 | 5.928 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.783 | -2.572 | 7.039 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.978 | -3.339 | 6.009 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.929 | -1.927 | 8.454 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23142.506 | -3.832 | 9.853 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23141.767 | -4.705 | 8.511 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23140.977 | -3.276 | 9.173 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23144.455 | -2.941 | 6.758 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23143.779 | -4.517 | 7.171 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23144.650 | -3.584 | 8.389 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.180 | -1.554 | 3.658 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.661 | -1.562 | 2.296 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.228 | -2.732 | 1.500 | 1.00 | 0.00 C |

| ATOM | 289 | O | ALA A | 24143.420 | -3.033 | 1.583 | 1.00 | 0.00 O |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 290 | CB | ALA A | 24141.979 | -0.245 | 1.603 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24143.104 | -1.837 | 3.819 | 1.00 | 0.00 H |
| ATOM | 292 | НА | ALA A | 24140.587 | -1.663 | 2.349 | 1.00 | 0.00 H |
| ATOM | 293 | IHB | ALA A | 24142.874 | -0.358 | 1.009 | 1.00 | 0.00 H |
| ATOM | 294 2 | 2HB | ALA A | 24142.134 | 0.524 | 2.345 | 1.00 | 0.00 H |
| ATOM | 295 3 | BHB | ALA A | 24141.155 | 0.033 | 0.962 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.369 | -3.388 | 0.727 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25141.786 | -4.526 | -0.084 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25141.885 | -4.138 | -1.555 | 1.00 | 0.00 C |
| ATOM | 299 | O | GLU A | 25140.962 | -3.548 | -2.117 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25140.802 | -5.686 | 0.084 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.261 | -6.974 | -0.579 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.550 | -7.240 | -1.891 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25140.211 | -8.414 | -2.155 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25140.330 | -6.277 | -2.654 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25140.432 | -3.101 | 0.703 | 1.00 | 0.00 H |
| ATOM | 306 | НА | GLU A | 25142.759 | -4.839 | 0.261 | 1.00 | 0.00 H |
| ATOM | 307 | lНВ | GLU A | 25140.665 | -5.878 | 1.138 | 1.00 | 0.00 H |
| ATOM | 308 2 | 2HB | GLU A | 25139.853 | -5.403 | -0.348 | 1.00 | 0.00 H |
| ATOM | 309 | IHG | GLU A | 25142.322 | -6.906 | -0.771 | 1.00 | 0.00 H |
| ATOM | 310 2 | 2HG | GLU A | 25141.069 | -7.798 | 0.092 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.013 | -4.472 | -2.175 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VALA | 26143.234 | -4.159 | -3.582 | 1.00 | 0.00 C |
| ATOM | 313 | C | VAL A | 26142.875 | -5.344 | -4.470 | 1.00 | 0.00 C |
| ATOM | 314 | Ο | VAL A | 26143.102 | -6.498 | -4.106 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VALA | 26144.698 | -3.759 | -3.844 | 1.00 | 0.00 C |

| ATOM | 316 | CG1 | VAL A | 26144.864 | -3.239 | -5.263 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 317 | CG2 | VAL A | 26145.159 | -2.722 | -2.830 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.712 | -4.941 | -1.674 | 1.00 | 0.00 H |
| ATOM | 319 | НА | VAL A | 26142.602 | -3.322 | -3.840 | 1.00 | 0.00 H |
| ATOM | 320 | НВ | VAL A | 26145.315 | -4.638 | -3.733 | 1.00 | 0.00 H |
| ATOM | 321 | lHG1 | VALA | 26143.919 | -2.852 | -5.618 | 1.00 | 0.00 H |
| ATOM | 322 2 | 2HG1 | VAL A | 26145.187 | -4.044 | -5.907 | 1.00 | 0.00 H |
| ATOM | 323 3 | 3HG1 | VAL A | 26145.602 | -2.450 | -5.274 | 1.00 | 0.00 H |
| ATOM | 324 1 | HG2 | VAL A | 26145.819 | -2.017 | -3.312 | 1.00 | 0.00 H |
| ATOM | 325 2 | 2HG2 | VAL A | 26145.683 | -3.214 | -2.026 | 1.00 | 0.00 H |
| ATOM | 326 3 | 3HG2 | VAL A | 26144.300 | -2.200 | -2.434 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYS A | 27142.313 | -5.052 | -5.639 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27141.922 | -6.094 | -6.581 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27143.099 | -6.503 | -7.462 | 1.00 | 0.00 C |
| ATOM | 330 | O | LYS A | 27143.028 | -6.423 | - 8.689 | 1.00 | 0.00 O |
| ATOM | 331 | CB | LYS A | 27140.758 | -5.616 | -7.450 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27139.941 | -6.748 | -8.051 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27138.455 | -6.426 | -8.056 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27138.093 | - 5.490 | -9.199 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27136.757 | -5.806 | -9.773 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27142.157 | -4.114 | -5.874 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27141.603 | -6.954 | -6.009 | 1.00 | 0.00 H |
| ATOM | 338 | lНВ | LYS A | 27140.100 | -5.008 | -6.846 | 1.00 | 0.00 H |
| ATOM | 339 2 | 2HB | LYS A | 27141.148 | -5.014 | -8.257 | 1.00 | 0.00 H |
| ATOM | 340 | IHG | LYSA | 27140.267 | -6.913 | -9.068 | 1.00 | 0.00 H |
| ATOM | 341 2 | 2HG | LYS A | 27140.104 | -7.644 | -7.470 | 1.00 | 0.00 H |
| ATOM | 342 | IHD | LYS A | 27137.898 | -7.344 | -8.166 | 1.00 | 0.00 H |

| ATOM | 343 | 2HD | LYS A | 27138.196 | -5.954 | -7.120 | 1.00 | 0.00 H |
|------|-----|-----|-------|-----------|-----------|---------|------|--------|
| ATOM | 344 | 1HE | LYS A | 27138.083 | -4.476 | -8.826 | 1.00 | 0.00 H |
| ATOM | 345 | 2HE | LYS A | 27138.840 | -5.581 | -9.973 | 1.00 | 0.00 H |
| ATOM | 346 | 1HZ | LYS A | 27136.863 | -6.410 - | 10.613 | 1.00 | 0.00 H |
| ATOM | 347 | 2HZ | LYS A | 27136.269 | -4.931 - | 10.049 | 1.00 | 0.00 H |
| ATOM | 348 | 3HZ | LYS A | 27136.175 | -6.307 | -9.072 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28144.182 | -6.941 | -6.829 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28145.374 | -7.363 | -7.554 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.422 | -8.882 | -7.682 | 1.00 | 0.00 C |
| ATOM | 352 | О | GLU A | 28144.507 | -9.581 | -7.248 | 1.00 | 0.00 O |
| ATOM | 353 | СВ | GLU A | 28146.634 | -6.857 | -6.845 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28147.639 | -6.209 | -7.782 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28148.605 | -5.292 | -7.057 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28148.525 | -4.063 | -7.264 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28149.440 | -5.803 | -6.282 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.179 | -6.982 | -5.849 | 1.00 | 0.00 H |
| ATOM | 359 | НА | GLU A | 28145.331 | -6.931 | -8.542 | 1.00 | 0.00 H |
| ATOM | 360 | 1HB | GLU A | 28146.346 | -6.129 | -6.102 | 1.00 | 0.00 H |
| ATOM | 361 | 2HB | GLU A | 28147.116 | -7.689 | -6.354 | 1.00 | 0.00 H |
| ATOM | 362 | 1HG | GLU A | 28148.206 | -6.984 | -8.275 | 1.00 | 0.00 H |
| ATOM | 363 | 2HG | GLU A | 28147.103 | -5.631 | -8.521 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29146.495 | -9.387 | -8.282 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29146.661 | -10.823 | -8.467 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29146.743 | -11.539 | -7.120 | 1.00 | 0.00 C |
| ATOM | 367 | Ο | ASN A | 29145.928 | -12.410 | -6.820 | 1.00 | 0.00 O |
| ATOM | 368 | СВ | ASN A | 29147.918 | -11.112 | -9.291 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29147.608 | -11.324 - | -10.760 | 1.00 | 0.00 C |

| ATOM | 370 OD1 ASN A | 29147.598 -12.454 - | 11.248 1.00 0.00 O |
|------|----------------|----------------------|--------------------|
| ATOM | 371 ND2 ASN A | 29147.356 -10.233 - | 11.475 1.00 0.00 N |
| ATOM | 372 H ASN A | 29147.192 -8.780 | -8.608 1.00 0.00 H |
| ATOM | 373 HA ASN A | 29145.798 -11.190 | -9.003 1.00 0.00 H |
| ATOM | 374 1HB ASN A | 29148.598 -10.277 | -9.203 1.00 0.00 H |
| ATOM | 375 2HB ASN A | 29148.395 -12.002 | -8.910 1.00 0.00 H |
| ATOM | 376 1HD2 ASN A | 29147.382 -9.365 - | 11.020 1.00 0.00 H |
| ATOM | 377 2HD2 ASN A | 29147.152 -10.341 -1 | 2.427 1.00 0.00 H |
| ATOM | 378 N PRO A | 30147.733 -11.175 | -6.287 1.00 0.00 N |
| ATOM | 379 CA PRO A | 30147.919 -11.784 | -4.967 1.00 0.00 C |
| ATOM | 380 C PRO A | 30146.921 -11.253 | -3.938 1.00 0.00 C |
| ATOM | 381 O PRO A | 30147.010 -10.099 | -3.519 1.00 0.00 O |
| ATOM | 382 CB PROA | 30149.341 -11.369 | -4.593 1.00 0.00 C |
| ATOM | 383 CG PROA | 30149.544 -10.067 | -5.286 1.00 0.00 C |
| ATOM | 384 CD PROA | 30148.751 -10.141 | -6.565 1.00 0.00 C |
| ATOM | 385 HA PROA | 30147.855 -12.860 | -5.014 1.00 0.00 H |
| ATOM | 386 1HB PRO A | 30149.419 -11.265 | -3.521 1.00 0.00 H |
| ATOM | 387 2HB PRO A | 30150.040 -12.115 | -4.942 1.00 0.00 H |
| ATOM | 388 1HG PRO A | 30149.181 -9.261 | -4.667 1.00 0.00 H |
| ATOM | 389 2HG PRO A | 30150.593 -9.927 | -5.506 1.00 0.00 H |
| ATOM | 390 1HD PRO A | 30148.285 -9.191 | -6.775 1.00 0.00 H |
| ATOM | 391 2HD PRO A | 30149.386 -10.439 | -7.385 1.00 0.00 H |
| ATOM | 392 N PRO A | 31145.956 -12.087 | -3.514 1.00 0.00 N |
| ATOM | 393 CA PROA | 31144.946 -11.687 | -2.529 1.00 0.00 C |
| ATOM | 394 C PRO A | 31145.541 -11.490 | -1.138 1.00 0.00 C |
| ATOM | 395 O PRO A | 31145.621 -12.431 | -0.349 1.00 0.00 O |
| ATOM | 396 CB PROA | 31143.962 -12.857 | -2.529 1.00 0.00 C |

| ATOM | 397 | CG | PRO A | 31144.764 | -14.027 | -2.981 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 398 | CD | PRO A | 31145.771 | -13.483 | -3.957 | 1.00 | 0.00 C |
| ATOM | 399 | НА | PRO A | 31144.436 | -10.783 | -2.831 | 1.00 | 0.00 H |
| ATOM | 400 1 | НВ | PRO A | 31143.574 | -13.006 | -1.531 | 1.00 | 0.00 H |
| ATOM | 401 2 | НВ | PRO A | 31143.149 | -12.649 | -3.209 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31145.264 | -14.479 | -2.137 | 1.00 | 0.00 H |
| ATOM | 403 2 | HG | PRO A | 31144.123 | -14.746 | -3.468 | 1.00 | 0.00 H |
| ATOM | 404 1 | HD | PRO A | 31146.697 | -14.035 | -3.889 | 1.00 | 0.00 H |
| ATOM | 405 2 | HD | PRO A | 31145.380 | -13.519 | -4.963 | 1.00 | 0.00 H |
| ATOM | 406 | N | PHE A | 32145.954 | -10.262 | -0.844 | 1.00 | 0.00 N |
| ATOM | 407 | CA | PHE A | 32146.541 | -9.942 | 0.452 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.685 | -8.925 | 1.201 | 1.00 | 0.00 C |
| ATOM | 409 | О | PHE A | 32144.726 | -8.383 | 0.652 | 1.00 | 0.00 O |
| ATOM | 410 | CB | PHE A | 32147.959 | -9.398 | 0.273 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.045 | -8.250 | -0.693 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.676 | -8.404 | -1.917 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32147.495 | -7.019 | -0.376 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.757 | -7.350 | -2.808 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.573 | -5.962 | -1.262 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.205 | -6.127 | -2.480 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.862 | -9.553 | -1.515 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.585 | -10.853 | 1.030 | 1.00 | 0.00 H |
| ATOM | 419 1 | НВ | PHE A | 32148.329 | -9.056 | 1.228 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.597 | -10.190 | -0.093 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32149.108 | -9.360 | -2.174 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32147.001 | -6.889 | 0.575 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32149.252 | -7.482 | -3.758 | 1.00 | 0.00 H |

| ATOM | 424 | HE2 | PHE A | 32147.140 | -5.006 | -1.004 | 1.00 | 0.00 H |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 425 | HZ | PHE A | 32148.266 | -5.302 | -3.174 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.038 | -8.673 | 2.456 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.302 | -7.722 | 3.281 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.253 | -6.758 | 3.983 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.107 | -7.174 | 4.765 | 1.00 | 0.00 O |
| ATOM | 430 | CB | TYR A | 33144.453 | -8.462 | 4.315 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.141 | -8.978 | 3.767 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.756 - | -10.298 | 3.963 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.290 | -8.145 | 3.051 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.559 - | 10.773 | 3.462 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.092 | -8.612 | 2.547 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.731 | -9.927 | 2.755 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.538 | -10.397 | 2.256 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.812 | -9.137 | 2.838 | 1.00 | 0.00 H |
| ATOM | 439 | НА | TYR A | 33144.650 | -7.156 | 2.632 | 1.00 | 0.00 H |
| ATOM | 440 1 | НВ | TYR A | 33145.010 | -9.308 | 4.690 | 1.00 | 0.00 H |
| ATOM | 441 2 | НВ | TYR A | 33144.231 | -7.793 | 5.134 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33143.406 | -10.958 | 4.516 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.577 | -7.116 | 2.889 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33141.276 - | -11.802 | 3.625 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.443 | -7.949 | 1.995 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.663 | -11.281 | 1.906 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34146.099 | -5.469 | 3.698 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.951 | -4.466 | 4.310 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34146.174 | -3.251 | 4.775 | 1.00 | 0.00 C |
| ATOM | 450 | O | GLY A | 34144.997 | -3.095 | 4.450 | 1.00 | 0.00 O |

| ATOM | 451 | Н | GLY A | 34145.401 | -5.196 | 3.066 | 1.00 | 0.00 H |
|------|-----|------|--------|-----------|---------|-------|------|--------|
| ATOM | 452 | 1HA | GLY A | 34147.453 | -4.907 | 5.160 | 1.00 | 0.00 H |
| ATOM | 453 | 2HA | GLY A | 34147.693 | -4.153 | 3.591 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.834 | -2.386 | 5.539 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VAL A | 35146.199 | -1.178 | 6.051 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.808 | 0.071 | 5.421 | 1.00 | 0.00 C |
| ATOM | 457 | 0 | VAL A | 35148.011 | 0.125 | 5.164 | 1.00 | 0.00 O |
| ATOM | 458 | СВ | VAL A | 35146.323 | -1.085 | 7.585 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.784 | -1.017 | 8.004 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VALA | 35145.552 | 0.115 | 8.113 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VALA | 35147.771 | -2.566 | 5.764 | 1.00 | 0.00 H |
| ATOM | 462 | HA | VAL A | 35145.150 | - 1.221 | 5.797 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.892 | -1.978 | 8.014 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VA'L A | 35148.204 | -0.071 | 7.695 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35148.330 | -1.823 | 7.536 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VAL A | 35147.856 | -1.109 | 9.077 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VAL A | 35145.807 | 0.279 | 9.150 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VAL A | 35144.492 | -0.072 | 8.028 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VAL A | 35145.810 | 0.992 | 7.536 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.971 | 1.073 | 5.176 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.429 | 2.321 | 4.577 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.374 | 3.064 | 5.516 | 1.00 | 0.00 C |
| ATOM | 473 | Ο | ILE A | 36147.092 | 3.216 | 6.705 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.246 | 3.243 | 4.222 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.208 | 2.484 | 3.392 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILEA | 36145.738 | 4.471 | 3.468 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.999 | 3.317 | 3.025 | 1.00 | 0.00 C |

| ATOM | 478 | Н | ILE A | 36145.024 | 0.971 | 5.403 | 1.00 | 0.00 H |
|------|-----|------|---------|-----------|-------|--------|--------|--------|
| ATOM | 479 | НА | ILE A | 36146.957 | 2.080 | 3.666 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.788 | 3.577 | 5.141 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.667 | 2.145 | 2.476 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.863 | 1.628 | 3.955 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36145.851 | 5.295 | 4.157 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36145.022 | 4.736 | 2.703 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36146.690 | 4.253 | 3.008 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36143.202 | 4.357 | 3.236 | 1.00 | 0.00 H |
| ATOM | 487 | 2HD1 | ILE A | 36142.148 | 2.992 | 3.605 | 1.00 | 0.00 H |
| ATOM | 488 | 3HD1 | ILE A | 36142.786 | 3.198 | 1.974 | 1.00 | 0.00 H |
| ATOM | 489 | N | ARG A | 37148.499 | 3.521 | 4.974 | 1.00 | 0.00 N |
| ATOM | 490 | CA | ARG A | 37149.487 | 4.246 | 5.763 | 1.00 | 0.00 C |
| ATOM | 491 | C | ARG A | 37149.637 | 5.680 | 5.265 | 1.00 | 0.00 C |
| ATOM | 492 | Ο | ARG A | 37149.354 | 6.632 | 5.992 | 1.00 | 0.00 O |
| ATOM | 493 | CB | ARG A | 37150.838 | 3.530 | 5.706 | 5 1.00 | 0.00 C |
| ATOM | 494 | CG | ARG A | 37150.753 | 2.046 | 6.021 | 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | 37150.195 | 1.803 | 7.414 | 1.00 | 0.00 C |
| ATOM | 496 | NE | ARG A | 37151.099 | 2.281 | 8.457 | 7 1.00 | 0.00 N |
| ATOM | 497 | CZ | ARG A | 37150.986 | 1.952 | 9.743 | 1.00 | 0.00 C |
| ATOM | 498 | NH1 | ARG A | 37150.012 | 1.148 | 10.146 | 1.00 | 0.00 N |
| ATOM | 499 | NH2 | 2 ARG A | 37151.853 | 2.429 | 10.626 | 1.00 | 0.00 N |
| ATOM | 500 | Н | ARG A | 37148.667 | 3.368 | 4.021 | 1.00 | 0.00 H |
| ATOM | 501 | HA | ARG A | 37149.145 | 4.267 | 6.787 | 7 1.00 | 0.00 H |
| ATOM | 502 | 1HB | ARG A | 37151.251 | 3.643 | 4.714 | 1.00 | 0.00 H |
| ATOM | 503 | 2HB | ARG A | 37151.507 | 3.990 | 6.419 | 1.00 | 0.00 H |
| ATOM | 504 | 1HG | ARG A | 37150.108 | 1.570 | 5.298 | 1.00 | 0.00 H |

| ATOM | 505 2 | HG | ARG A | 37151.743 | 1.618 | 5.960 | 1.00 | 0.00 H | |
|------|-------|--------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 506 1 | HD | ARG A | 37149.251 | 2.321 | 7.505 | 1.00 | 0.00 H | |
| ATOM | 507 2 | 2HD | ARG A | 37150.037 | 0.742 | 7.545 | 1.00 | 0.00 H | |
| ATOM | 508 | HE | ARG A | 37151.828 | 2.877 | 8.187 | 1.00 | 0.00 H | |
| ATOM | 509 1 | HH1. | ARG A | 37149.355 | 0.785 | 9.486 | 1.00 | 0.00 H | |
| ATOM | 510 2 | HH1. | ARG A | 37149.933 | 0.905 | 11.114 | 1.00 | 0.00 H | |
| ATOM | 511 1 | нн2 | ARG A | 37152.590 | 3.035 | 10.327 | 1.00 | 0.00 H | |
| ATOM | 512 2 | 2HH2 . | ARG A | 37151.769 | 2.182 | 11.592 | 1.00 | 0.00 H | |
| ATOM | 513 | N | TRP A | 38150.084 | 5.827 | 4.022 | 1.00 | 0.00 N | |
| ATOM | 514 | CA | TRP A | 38150.270 | 7.146 | 3.428 | 1.00 | 0.00 C | |
| ATOM | 515 | C | TRP A | 38149.501 | 7.268 | 2.117 | 1.00 | 0.00 C | |
| ATOM | 516 | O | TRP A | 38149.565 | 6.385 | 1.262 | 1.00 | 0.00 O | |
| ATOM | 517 | CB | TRP A | 38151.761 | 7.418 | 3.190 | 1.00 | 0.00 C | |
| ATOM | 518 | CG | TRPA | 38152.021 | 8.634 | 2.350 | 1.00 | 0.00 C | |
| ATOM | 519 | CD1 | TRP A | 38152.212 | 9.911 | 2.791 | 1.00 | 0.00 C | |
| ATOM | 520 | CD2 | TRP A | 38152.116 | 8.683 | 0.922 | 1.00 | 0.00 C | |
| ATOM | 521 | NE1 | TRPA | 38152.417 | 10.753 | 1.725 | 1.00 | 0.00 N | |
| ATOM | 522 | CE2 | TRPA | 38152.363 | 10.022 | 0.565 | 1.00 | 0.00 C | |
| ATOM | 523 | CE3 | TRPA | 38152.014 | 7.725 | -0.090 | 1.00 | 0.00 C | |
| ATOM | 524 | CZ2 | TRPA | 38152.511 | 10.424 | -0.760 | 1.00 | 0.00 C | |
| ATOM | 525 | CZ3 | TRPA | 38152.162 | 8.125 | -1.405 | 1.00 | 0.00 C | |
| ATOM | 526 | CH2 | TRP A | 38152.408 | 9.465 | -1.729 | 1.00 | 0.00 C | |
| ATOM | 527 | Н | TRPA | 38150.293 | 5.030 | 3.491 | 1.00 | 0.00 H | |
| ATOM | 528 | HA | TRPA | 38149.888 | 7.879 | 4.123 | 1.00 | 0.00 H | |
| ATOM | 529 1 | lНВ | TRPA | 38152.250 | 7.560 | 4.142 | 1.00 | 0.00 H | |
| ATOM | 530 2 | 2HB | TRPA | 38152.198 | 6.566 | 2.690 | 1.00 | 0.00 H | |
| ATOM | 531 | HD1 | TRPA | 38152.198 | 10.204 | 3.831 | 1.00 | 0.00 H | |

| ATOM | 532 | HE1 | TRPA | 38152.577 | 11.718 | 1.783 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 533 | HE3 | TRPA | 38151.825 | 6.687 | 0.140 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38152.699 | 11.454 | -1.027 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.087 | 7.398 | -2.200 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRPA | 38152.516 | 9.733 | -2.771 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.781 | 8.374 | 1.963 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39148.004 | 8.624 | 0.756 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILE A | 39148.406 | 9.950 | 0.121 | 1.00 | 0.00 C |
| ATOM | 540 | О | ILE A | 39148.069 | 11.019 | 0.631 | 1.00 | 0.00 O |
| ATOM | 541 | CB | ILE A | 39146.492 | 8.645 | 1.051 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39146.088 | 7.406 | 1.853 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.699 | 8.725 | -0.245 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.772 | 7.560 | 2.583 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.776 | 9.043 | 2.680 | 1.00 | 0.00 H |
| ATOM | 546 | HA | ILE A | 39148.205 | 7.824 | 0.056 | 1.00 | 0.00 H |
| ATOM | 547 | HB | ILE A | 39146.274 | 9.527 | 1.633 | 1.00 | 0.00 H |
| ATOM | 548 | 1HG1 | ILE A | 39145.997 | 6.564 | 1.182 | 1.00 | 0.00 H |
| ATOM | 549 | 2HG1 | ILE A | 39146.852 | 7.195 | 2.587 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39144.687 | 9.034 | -0.029 | 1.00 | 0.00 H |
| ATOM | 551 | 2HG2 | ILE A | 39145.686 | 7.756 | -0.720 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39146.162 | 9.443 | -0.905 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.751 | 8.514 | 3.089 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39144.666 | 6.766 | 3.306 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39143.960 | 7.512 | 1.874 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.135 | 9.876 | -0.987 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.575 | 11.083 | -1.663 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.097 | 10.816 | -3.060 | 1.00 | 0.00 C |

| ATOM | 559 | O | GLY A | 40149.921 | 9.724 | -3.600 | 1.00 | 0.00 O |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 560 | Н | GLY A | 40149.378 | 8.997 | -1.348 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40148.745 | 11.769 | -1.727 | 1.00 | 0.00 H |
| ATOM | 562 2 | 2HA | GLY A | 40150.359 | 11.540 | -1.079 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41150.741 | 11.820 | -3.644 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.294 | 11.701 | -4.987 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41152.768 | 12.102 | -5.001 | 1.00 | 0.00 C |
| ATOM | 566 | O | GLN A | 41153.105 | 13.259 | -4.749 | 1.00 | 0.00 O |
| ATOM | 567 | СВ | GLN A | 41150.504 | 12.581 | -5.956 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41148.998 | 12.402 | -5.849 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.246 | 13.712 | -5.972 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.223 | 14.518 | -5.040 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41147.627 | 13.933 | -7.125 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41150.847 | 12.665 | -3.160 | 1.00 | 0.00 H |
| ATOM | 573 | НА | GLN A | 41151.205 | 10.672 | -5.295 | 1.00 | 0.00 H |
| ATOM | 574 | 1HB | GLN A | 41150.737 | 13.616 | -5.753 | 1.00 | 0.00 H |
| ATOM | 575 2 | 2HB | GLN A | 41150.804 | 12.344 | -6.964 | 1.00 | 0.00 H |
| ATOM | 576 | 1HG | GLN A | 41148.670 | 11.741 | -6.637 | 1.00 | 0.00 H |
| ATOM | 577 2 | 2HG | GLN A | 41148.767 | 11.960 | -4.891 | 1.00 | 0.00 H |
| ATOM | 578 | 1HE2 | GLN A | 41147.689 | 13.246 | -7.822 | 1.00 | 0.00 H |
| ATOM | 579 2 | 2HE2 | GLN A | 41147.135 | 14.773 | -7.233 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42153.674 | 11.150 | -5.295 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.115 | 11.422 | -5.336 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.468 | 12.529 | -6.324 | 1.00 | 0.00 C |
| ATOM | 583 | O | PRO A | 42154.696 | 12.830 | -7.233 | 1.00 | 0.00 O |
| ATOM | 584 | СВ | PRO A | 42155.723 | 10.089 | -5.787 | 1.00 | 0.00 C |
| ATOM | 585 | CG | PRO A | 42154.699 | 9.066 | -5.440 | 1.00 | 0.00 C |

| ATOM | 586 CD | PRO A | 42153.371 | 9.743 | - 5.609 | 1.00 | 0.00 C |
|------|---------|-------|-----------|----------|---------|------|--------|
| ATOM | 587 HA | PRO A | 42155.495 | 11.680 | -4.358 | 1.00 | 0.00 H |
| ATOM | 588 1HB | PRO A | 42155.909 | 10.118 | -6.851 | 1.00 | 0.00 H |
| ATOM | 589 2HB | PRO A | 42156.648 | 9.915 | -5.259 | 1.00 | 0.00 H |
| ATOM | 590 1HG | PRO A | 42154.778 | 8.222 | -6.110 | 1.00 | 0.00 H |
| ATOM | 591 2HG | PRO A | 42154.830 | 8.746 | -4.416 | 1.00 | 0.00 H |
| ATOM | 592 1HD | PRO A | 42153.021 | 9.641 | -6.626 | 1.00 | 0.00 H |
| ATOM | 593 2HD | PRO A | 42152.648 | 9.341 | -4.916 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43156.647 | 13.151 | -6.158 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.102 | 14.228 | -7.040 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43157.497 | 13.719 | -8.421 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43158.662 | 13.408 | -8.668 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43158.322 | 14.792 | -6.312 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43158.835 | 13.657 | -5.497 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43157.629 | 12.850 | -5.098 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43156.351 | 14.999 | -7.142 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43159.052 | 15.121 | -7.037 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43158.023 | 15.622 | -5.691 | 1.00 | 0.00 H |
| ATOM | 604 1HG | PRO A | 43159.510 | 13.056 | -6.088 | 1.00 | 0.00 H |
| ATOM | 605 2HG | PRO A | 43159.339 | 14.035 | -4.619 | 1.00 | 0.00 H |
| ATOM | 606 1HD | PRO A | 43157.869 | 11.797 | -5.082 | 1.00 | 0.00 H |
| ATOM | 607 2HD | PRO A | 43157.264 | 13.170 | -4.134 | 1.00 | 0.00 H |
| ATOM | 608 N | GLY A | 44156.521 | 13.636 | -9.317 | 1.00 | 0.00 N |
| ATOM | 609 CA | GLY A | 44156.790 | 13.162 | -10.661 | 1.00 | 0.00 C |
| ATOM | 610 C | GLY A | 44155.552 | 12.623 - | 11.346 | 1.00 | 0.00 C |
| ATOM | 611 O | GLY A | 44155.237 | 13.014 - | 12.471 | 1.00 | 0.00 O |
| ATOM | 612 H | GLY A | 44155.610 | 13.897 | -9.064 | 1.00 | 0.00 H |

| ATOM | 613 | 1HA | GLY A | 44157.183 | 13.980 -11.245 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|----------------|------|--------|
| ATOM | 614 | 2HA | GLY A | 44157.532 | 12.380 -10.613 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45154.848 | 11.724 -10.670 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEU A | 45153.637 | 11.131 -11.224 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45152.440 | 11.401 -10.319 | 1.00 | 0.00 C |
| ATOM | 618 | О | LEU A | 45152.369 | 10.888 -9.203 | 1.00 | 0.00 O |
| ATOM | 619 | СВ | LEU Å | 45153.820 | 9.623 -11.409 | 1.00 | 0.00 C |
| ATOM | 620 | CG | LEU A | 45154.384 | 8.886 -10.192 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.025 | 7.407 -10.247 | 1.00 | 0.00 C |
| ATOM | 622 | CD2 | LEU A | 45155.893 | 9.072 -10.107 | 1.00 | 0.00 C |
| ATOM | 623 | Н | LEU A | 45155.148 | 11.452 -9.775 | 1.00 | 0.00 H |
| ATOM | 624 | НА | LEU A | 45153.455 | 11.583 -12.186 | 1.00 | 0.00 H |
| ATOM | 625 | 1HB | LEU A | 45152.860 | 9.192 -11.653 | 1.00 | 0.00 H |
| ATOM | 626 | 2HB | LEU A | 45154.490 | 9.462 -12.240 | 1.00 | 0.00 H |
| ATOM | 627 | HG | LEU A | 45153.945 | 9.301 -9.295 | 1.00 | 0.00 H |
| ATOM | 628 | 1HD1 | LEU A | 45153.490 | 7.134 -9.349 | 1.00 | 0.00 H |
| ATOM | 629 | 2HD1 | LEU A | 45154.928 | 6.819 -10.320 | 1.00 | 0.00 H |
| ATOM | 630 | 3HD1 | LEU A | 45153.402 | 7.218 -11.108 | 1.00 | 0.00 H |
| ATOM | 631 | 1HD2 | LEU A | 45156.162 | 9.381 -9.108 | 1.00 | 0.00 H |
| ATOM | 632 | 2HD2 | LEU A | 45156.205 | 9.827 -10.813 | 1.00 | 0.00 H |
| ATOM | 633 | 3HD2 | LEU A | 45156.385 | 8.138 -10.339 | 1.00 | 0.00 H |
| ATOM | 634 | N | ASN A | 46151.505 | 12.210 -10.803 | 1.00 | 0.00 N |
| ATOM | 635 | CA | ASN A | 46150.318 | 12.539 -10.025 | 1.00 | 0.00 C |
| ATOM | 636 | C | ASN A | 46149.367 | 11.349 -9.971 | 1.00 | 0.00 C |
| ATOM | 637 | Ο | ASN A | 46148.723 | 11.008 -10.964 | 1.00 | 0.00 O |
| ATOM | 638 | СВ | ASN A | 46149.608 | 13.751 -10.630 | 1.00 | 0.00 C |
| ATOM | 639 | CG | ASN A | 46148.879 | 14.574 -9.586 | 1.00 | 0.00 C |

| ATOM | 640 | OD1 | ASN A | 46147.654 | 14.691 | -9.615 | 1.00 | 0.00 O |
|------|-------|------|-------|-----------|----------|---------|------|--------|
| ATOM | 641 | ND2 | ASN A | 46149.632 | 15.152 | -8.657 | 1.00 | 0.00 N |
| ATOM | 642 | Н | ASN A | 46151.613 | 12.592 | -11.699 | 1.00 | 0.00 H |
| ATOM | 643 | HA | ASN A | 46150.633 | 12.780 | -9.020 | 1.00 | 0.00 H |
| ATOM | 644 | 1HB | ASN A | 46150.337 | 14.383 - | -11.114 | 1.00 | 0.00 H |
| ATOM | 645 2 | 2HB | ASN A | 46148.889 | 13.411 - | 11.361 | 1.00 | 0.00 H |
| ATOM | 646 | 1HD2 | ASN A | 46150.602 | 15.015 | -8.696 | 1.00 | 0.00 H |
| ATOM | 647 2 | 2HD2 | ASN A | 46149.188 | 15.690 | -7.970 | 1.00 | 0.00 H |
| ATOM | 648 | N | GLU A | 47149.285 | 10.721 | -8.804 | 1.00 | 0.00 N |
| ATOM | 649 | CA | GLU A | 47148.415 | 9.568 | -8.612 | 1.00 | 0.00 C |
| ATOM | 650 | C | GLU A | 47148.262 | 9.248 | -7.130 | 1.00 | 0.00 C |
| ATOM | 651 | О | GLU A | 47149.245 | 8.978 | -6.440 | 1.00 | 0.00 O |
| ATOM | 652 | CB | GLU A | 47148.970 | 8.349 | -9.354 | 1.00 | 0.00 C |
| ATOM | 653 | CG | GLU A | 47150.485 | 8.230 | -9.290 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.036 | 7.254 | -10.311 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.168 | 7.641 - | -11.491 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.336 | 6.103 | -9.930 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47149.824 | 11.041 | -8.052 | 1.00 | 0.00 H |
| ATOM | 658 | HA | GLU A | 47147.445 | 9.813 | -9.017 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.543 | 7.455 | -8.923 | 1.00 | 0.00 H |
| ATOM | 660 2 | 2HB | GLU A | 47148.680 | 8.411 | -10.392 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47150.917 | 9.201 | -9.474 | 1.00 | 0.00 H |
| ATOM | 662 2 | 2HG | GLU A | 47150.767 | 7.894 | -8.303 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.026 | 9.273 | -6.644 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VALA | 48146.758 | 8.977 | -5.243 | 1.00 | 0.00 C |
| ATOM | 665 | C | VAL A | 48147.120 | 7.533 | -4.918 | 1.00 | 0.00 C |
| ATOM | 666 | О | VAL A | 48146.338 | 6.615 | -5.169 | 1.00 | 0.00 O |

| ATOM | 667 | CB | VAL A | 48145.279 | 9.219 | -4.888 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 668 | CG1 | VALA | 48145.066 | 9.114 | -3.386 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VAL A | 48144.820 | 10.574 | -5.405 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.280 | 9.489 | -7.241 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.366 | 9.636 | -4.640 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48144.684 | 8.455 | -5.368 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48145.014 | 8.072 | -3.102 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VAL A | 48144.142 | 9.606 | -3.117 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48145.889 | 9.587 | -2.872 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48144.651 | 10.515 | -6.470 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48145.580 | 11.314 | -5.202 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VAL A | 48143.903 | 10.857 | -4.910 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.309 | 7.339 | -4.362 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49148.777 | 6.005 | -4.005 | 1.00 | 0.00 C |
| ATOM | 681 | C | LEU A | 49148.742 | 5.809 | -2.496 | 1.00 | 0.00 C |
| ATOM | 682 | ·O | LEU A | 49149.455 | 6.486 | -1.756 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.197 | 5.781 | -4.528 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.343 | 5.837 | -6.050 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49151.745 | 6.281 | -6.435 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEUA | 49150.022 | 4.483 | -6.664 | 1.00 | 0.00 C |
| ATOM | 687 | Н | LEU A | 49148.888 | 8.110 | -4.186 | 1.00 | 0.00 H |
| ATOM | 688 | HA | LEU A | 49148.115 | 5.287 | -4.466 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49150.840 | 6.535 | -4.097 | 1.00 | 0.00 H |
| ATOM | 690 | 2HB | LEU A | 49150.532 | 4.812 | -4.192 | 1.00 | 0.00 H |
| ATOM | 691 | HG | LEU A | 49149.643 | 6.559 | -6.446 | 1.00 | 0.00 H |
| ATOM | 692 | 1HD1 | LEU A | 49151.964 | 7.230 | -5.968 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49151.808 | 6.384 | -7.507 | 1.00 | 0.00 H |

| ATOM | 694 3 | 3HD1 | LEU A | 49152.461 | 5.543 | -6.102 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 695 | 1HD2 | LEU A | 49149.950 | 4.582 | -7.737 | 1.00 | 0.00 H |
| ATOM | 696 2 | 2HD2 | LEU A | 49149.083 | 4.122 | -6.272 | 1.00 | 0.00 H |
| ATOM | 697 | 3HD2 | LEU A | 49150.807 | 3.782 | -6.420 | 1.00 | 0.00 H |
| ATOM | 698 | N | ALA A | 50147.908 | 4.880 | -2.044 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.783 | 4.602 | -0.621 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALA A | 50148.733 | 3.488 | -0.195 | 1.00 | 0.00 C |
| ATOM | 701 | O | ALA A | 50148.596 | 2.343 | -0.625 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.347 | 4.234 | -0.280 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.363 | 4.374 | -2.682 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50148.036 | 5.505 | -0.086 | 1.00 | 0.00 H |
| ATOM | 705 | lНВ | ALA A | 50146.227 | 3.162 | -0.329 | 1.00 | 0.00 H |
| ATOM | 706 2 | 2HB | ALA A | 50145.677 | 4.704 | -0.985 | 1.00 | 0.00 H |
| ATOM | 707 | ЗНВ | ALA A | 50146.115 | 4.577 | 0.718 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.697 | 3.832 | 0.653 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.656 | 2.850 | 1.123 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51150.023 | 1.805 | 2.019 | 1.00 | 0.00 C |
| ATOM | 711 | O | GLY A | 51149.665 | 2.092 | 3.162 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.757 | 4.759 | 0.962 | 1.00 | 0.00 H |
| ATOM | 713 | lНА | GLY A | 51151.098 | 2.357 | 0.270 | 1.00 | 0.00 H |
| ATOM | 7142 | 2HA | GLY A | 51151.434 | 3.357 | 1.674 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.882 | 0.589 | 1.501 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.286 | -0.502 | 2.264 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.362 | -1.350 | 2.933 | 1.00 | 0.00 C |
| ATOM | 718 | О | LEU A | 52151.348 | - 1.734 | 2.303 | 1.00 | 0.00 O |
| ATOM | ,719 | CB | LEU A | 52148.423 | -1.376 | 1.353 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.132 | -0.721 | 0.860 | 1.00 | 0.00 C |

0.00 C **ATOM** CD1 LEU A 52146.434 -1.615 -0.154 1.00 721 **ATOM** CD2 LEU A 52146.209 -0.418 2.031 1.00 0.00 C 722 **ATOM** Η LEUA 52150.186 0.422 0.585 1.00 0.00 H 723 **ATOM** HA LEUA 52148.660 -0.067 3.029 1.00 0.00 H 724 **ATOM** 725 1HB LEUA 52149.014 -1.654 0.492 1.00 0.00 H **ATOM** 726 2HB LEU A 52148.162 -2.274 1.893 1.00 0.00 H **ATOM** 727 HG LEUA 52147.372 0.212 0.373 1.00 0.00 H **ATOM** 728 1HD1 LEU A 52147.160 -2.260 -0.625 1.00 0.00 H **ATOM** 729 2HD1 LEU A 52145.957 -1.002 -0.905 1.00 0.00 H**ATOM** 730 3HD1 LEU A 52145.689 -2.215 0.348 1.00 0.00 H**ATOM** 731 1HD2 LEU A 52146.708 0.245 2.721 1.00 0.00 H **ATOM** 732 2HD2 LEU A 52145.955 -1.339 2.536 1.00 0.00 H**ATOM** 733 3HD2 LEU A 52145.308 0.053 1.666 1.00 0.00 H 734 N GLU A 53150.166 -1.641 4.216 1.00 0.00 N **ATOM** CA GLUA 53151.119 -2.445 4.972 1.00 0.00 C **ATOM** 735 1.00 **ATOM** 736 C GLUA 53150.624 -3.880 5.117 0.00 C GLUA 53149.715 -4.158, 1.00 0.00 O **ATOM** 737 O 5.899 **ATOM** CB GLUA 53151.353 -1.830 6.353 1.00 0.00 C 738 1.00 0.00 C **ATOM** 739 CG GLUA 53152.363 -2.593 7.195 1.00 0.00 C **ATOM** 740 CD GLUA 53151.997 -2.614 8.666 **ATOM** 741 OE1 GLU A 53152.380 -3.580 9.360 1.00 0.00 O 1.00 **ATOM** 742 OE2 GLU A 53151.327 -1.665 9.126 0.00 O **ATOM** 743 Η GLUA 53149.362 -1.306 4.663 1.00 0.00 H **ATOM** 744 HA GLUA 53152.053 -2.451 4.428 1.00 0.00 H 6.229 1.00 0.00 H**ATOM** 745 1HB GLUA 53151.710 -0.819 6.887 1.00 0.00 H**ATOM** 746 2HB GLUA 53150.414 -1.808 6.838 1.00 0.00 H **ATOM** 747 1HG GLUA 53152.415 -3.610

| ATOM | 748 | 2HG | GLU A | 53153.330 | -2.124 | 7.086 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 749 | N | LEU A | 54151.229 | -4.789 | 4.359 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.850 | -6.196 | 4.403 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54151.179 | -6.805 | 5.763 | 1.00 | 0.00 C |
| ATOM | 752 | O | LEU A | 54152.268 | -6.599 | 6.300 | 1.00 | 0.00 O |
| ATOM | 753 | CB | LEU A | 54151.564 | -6.973 | 3.296 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.397 | -6.396 | 1.889 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.493 | -6.907 | 0.968 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54150.025 | -6.742 | 1.331 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.948 | -4.506 | 3.755 | 1.00 | 0.00 H |
| ATOM | 758 | HA | LEU A | 54149.784 | -6.257 | 4.244 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.618 | -7.003 | 3.529 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54151.183 | -7.984 | 3.293 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.478 | -5.319 | 1.938 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54153.458 | -6.635 | 1.372 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54152.376 | -6.467 | -0.011 | 1.00 | 0.00 H |
| ATOM | 764 | 3HD1 | LEU A | 54152.426 | -7.982 | 0.891 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54149.885 | -7.812 | 1.357 | 1.00 | 0.00 H |
| ATOM | 766 | 2HD2 | LEU A | 54149.953 | -6.394 | 0.312 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.262 | -6.266 | 1.929 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55150.231 | -7.556 | 6.314 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55150.420 | -8.196 | 7.610 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55151.540 | -9.230 | 7.551 | 1.00 | 0.00 C |
| ATOM | 771 | Ο | GLU A | 55152.232 | -9.466 | 8.542 | 1.00 | 0.00 O |
| ATOM | 772 | CB | GLU A | 55149.120 | -8.861 | 8.068 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55148.144 | -7.900 | 8.725 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55148.143 | -8.013 | 10.237 | 1.00 | 0.00 C |

| ATOM | 775 | OE1 | GLU A | 55149.238 | -7.979 | 10.837 | 1.00 | 0.00 O |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 776 | OE2 | GLU A | 55147.046 | -8.137 | 10.823 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.385 | -7.684 | 5.837 | 1.00 | 0.00 H |
| ATOM | 778 | НА | GLU A | 55150.690 | -7.429 | 8.321 | 1.00 | 0.00 H |
| ATOM | 779 1 | НВ | GLU A | 55148.635 | -9.303 | 7.210 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55149.358 | -9.639 | 8.778 | 1.00 | 0.00 H |
| ATOM | 781 1 | HG | GLU A | 55148.415 | -6.890 | 8.457 | 1.00 | 0.00 H |
| ATOM | 782 2 | HG | GLU A | 55147.148 | -8.113 | 8.362 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASP A | 56151.713 | -9.843 | 6.385 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASPA | 56152.748 - | 10.852 | 6.199 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASP A | 56153.972 - | 10.256 | 5.509 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASPA | 56153.857 | -9.318 | 4.722 | 1.00 | 0.00 O |
| ATOM | 787 | CB | ASPA | 56152.207 - | 12.024 | 5.379 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56152.759 - | 13.358 | 5.842 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASPA | 56152.112 - | 14.007 | 6.689 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56153.839 - | 13.754 | 5.355 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56151.130 | -9.612 | 5.632 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56153.040 - | -11.212 | 7.174 | 1.00 | 0.00 H |
| ATOM | 793 1 | НВ | ASPA | 56151.131 - | 12.052 | 5.468 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASPA | 56152.474 - | 11.884 | 4.341 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57155.142 | -10.810 | 5.811 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57156.387 | -10.334 | 5.219 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.650 | -11.019 | 3.882 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57156.986 | -12.203 | 3.836 | 1.00 | 0.00 O |
| ATOM | 799 | СВ | GLU A | 57157.558 | -10.584 | 6.172 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.490 | -9.760 | 7.448 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57158.429 | -10.272 | 8.522 | 1.00 | 0.00 C |

| ATOM | 802 | OE1 | GLU A | 57159.608 - | 10.536 | 8.205 | 1.00 | 0.00 O |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 803 | OE2 | GLU A | 57157.985 - | 10.409 | 9.682 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57155.169 | -11.556 | 6.445 | 1.00 | 0.00 H |
| ATOM | 805 | HA | GLU A | 57156.291 | -9.272 | 5.053 | 1.00 | 0.00 H |
| ATOM | 806 1 | HB | GLU A | 57157.567 | -11.629 | 6.445 | 1.00 | 0.00 H |
| ATOM | 807 2 | HB | GLU A | 57158.480 | -10.345 | 5.663 | 1.00 | 0.00 H |
| ATOM | 808 1 | HG | GLU A | 57157.756 | -8.740 | 7.216 | 1.00 | 0.00 H |
| ATOM | 809 2 | HG | GLU A | 57156.480 | -9.791 | 7.828 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58156.495 - | 10.269 | 2.797 | 1.00 | 0.00 N |
| ATOM | 811 | CA | CYS A | 58156.716 | -10.804 | 1.459 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58157.997 - | 10.242 | 0.851 | 1.00 | 0.00 C |
| ATOM | 813 | O | CYS A | 58158.317 | -9.067 | 1.030 | 1.00 | 0.00 O |
| ATOM | 814 | CB | CYS A | 58155.524 | -10.482 | 0.554 | 1.00 | 0.00 C |
| ATOM | 815 | SG | CYS A | 58154.176 | -11.683 | 0.653 | 1.00 | 0.00 S |
| ATOM | 816 | Н | CYS A | 58156.226 | -9.331 | 2.898 | 1.00 | 0.00 H |
| ATOM | 817 | НА | CYS A | 58156.812 | -11.877 | 1.542 | 1.00 | 0.00 H |
| ATOM | 818 1 | HB | CYS A | 58155.125 | -9.517 | 0.830 | 1.00 | 0.00 H |
| ATOM | 819 2 | НВ | CYS A | 58155.861 - | 10.447 | -0.472 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYSA | 58154.554 | -12.533 | 0.888 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALA A | 59158.726 | -11.089 | 0.133 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALA A | 59159.972 | -10.677 | -0.502 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59159.708 | -9.725 | -1.664 | 1.00 | 0.00 C |
| ATOM | 824 | О | ALA A | 59159.129 | -10.113 | -2.678 | 1.00 | 0.00 O |
| ATOM | 825 | CB | ALA A | 59160.747 | -11.895 | -0.981 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALA A | 59158.418 | -12.014 | 0.026 | 1.00 | 0.00 H |
| ATOM | 827 | НА | ALA A | 59160.570 | -10.168 | 0.239 | 1.00 | 0.00 H |
| ATOM | 828 1 | HB | ALA A | 59161.352 - | 11.625 | -1.834 | 1.00 | 0.00 H |

| ATOM | 829 2 | 2HB | ALA A | 59160.054 | -12.674 | -1.265 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 830 3 | ЗНВ | ALA A | 59161.385 | -12.252 | -0.186 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60160.136 | -8.476 | -1.508 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60159.937 | -7.489 | -2.551 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60159.402 | -6.175 | -2.012 | 1.00 | 0.00 C |
| ATOM | 834 | O | GLY A | 60159.649 | -5.115 | -2.587 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60160.591 | -8.225 | -0.677 | 1.00 | 0.00 H |
| ATOM | 836 | lHA | GLY A | 60160.880 | -7.305 | -3.044 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60159.236 | -7.880 | -3.274 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61158.669 | -6.247 | -0.907 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.098 | -5.055 | -0.290 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.175 | -4.242 | 0.422 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.259 | -4.749 | 0.712 | 1.00 | 0.00 O |
| ATOM | 842 | CB | CYS A | 61156.999 | -5.444 | 0.700 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYSA | 61155.806 | -6.635 | 0.046 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.508 | -7.121 | -0.495 | 1.00 | 0.00 H |
| ATOM | 845 | HA | CYSA | 61157.667 | -4.450 | -1.074 | 1.00 | 0.00 H |
| ATOM | 846 | IHB | CYS A | 61157.452 | - 5.882 | 1.576 | 1.00 | 0.00 H |
| ATOM | 847 2 | 2HB | CYS A | 61156.453 | -4.556 | 0.988 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61156.257 | -7.181 | -0.602 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.869 | -2.979 | 0.700 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.811 | -2.096 | 1.378 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.450 | -1.944 | 2.852 | 1.00 | 0.00 C |
| ATOM | 852 | О | THR A | 62158.508 | -2.571 | 3.338 | 1.00 | 0.00 O |
| ATOM | 853 | СВ | THR A | 62159.834 | -0.725 | 0.702 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.569 | -0.422 | 0.140 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.865 | -0.617 | -0.400 | 1.00 | 0.00 C |

| ATOM | 856 | Н | THR A | 62157.989 | -2.632 | 0.443 | 1.00 | 0.00 H | |
|------|-----|------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 857 | НА | THR A | 62160.793 | -2.540 | 1.305 | 1.00 | 0.00 H | |
| ATOM | 858 | HB | THR A | 62160.063 | 0.027 | 1.444 | 1.00 | 0.00 H | |
| ATOM | 859 | HG1 | THR A | 62158.577 | 0.476 | -0.200 | 1.00 | 0.00 H | |
| ATOM | 860 | 1HG2 | THR A | 62161.107 | 0.422 | -0.567 | 1.00 | 0.00 H | |
| ATOM | 861 | 2HG2 | THR A | 62160.466 | -1.044 | -1.309 | 1.00 | 0.00 H | |
| ATOM | 862 | 3HG2 | THR A | 62161.757 | -1.153 | -0.112 | 1.00 | 0.00 H | |
| ATOM | 863 | N | ASPA | 63160.204 | -1.108 | 3.557 | 1.00 | 0.00 N | |
| ATOM | 864 | CA | ASPA | 63159.963 | -0.873 | 4.977 | 1.00 | 0.00 C | |
| ATOM | 865 | C | ASPA | 63159.263 | 0.463 | 5.197 | 1.00 | 0.00 C | |
| ATOM | 866 | Ο | ASPA | 63159.501 | 1.144 | 6.194 | 1.00 | 0.00 O | |
| ATOM | 867 | CB | ASP A | 63161.283 | -0.905 | 5.752 | 1.00 | 0.00 C | |
| ATOM | 868 | CG | ASPA | 63162.354 | -0.050 | 5.104 | 1.00 | 0.00 C | |
| ATOM | 869 | OD1 | ASP A | 63163.372 | -0.615 | 4.652 | 1.00 | 0.00 O | |
| ATOM | 870 | OD2 | ASPA | 63162.175 | 1.185 | 5.048 | 1.00 | 0.00 O | |
| ATOM | 871 | Н | ASPA | 63160.940 | -0.637 | 3.114 | 1.00 | 0.00 H | |
| ATOM | 872 | НА | ASPA | 63159.324 | -1.665 | 5.339 | 1.00 | 0.00 H | |
| ATOM | 873 | 1HB | ASPA | 63161.114 | -0.538 | 6.753 | 1.00 | 0.00 H | |
| ATOM | 874 | 2HB | ASPA | 63161.640 | -1.922 | 5.800 | 1.00 | 0.00 H | |
| ATOM | 875 | N | GLY A | 64158.398 | 0.833 | 4.258 | 1.00 | 0.00 N | |
| ATOM | 876 | CA | GLY A | 64157.676 | 2.087 | 4.367 | 1.00 | 0.00 C | |
| ATOM | 877 | C | GLY A | 64158.318 | 3.199 | 3.562 | 1.00 | 0.00 C | |
| ATOM | 878 | О | GLY A | 64158.413 | 4.336 | 4.025 | 1.00 | 0.00 O | |
| ATOM | 879 | Н | GLY A | 64158.249 | 0.250 | 3.485 | 1.00 | 0.00 H | |
| ATOM | 880 | 1HA | GLY A | 64156.666 | 1.940 | 4.016 | 1.00 | 0.00 H | |
| ATOM | 881 | 2HA | GLY A | 64157.644 | 2.382 | 5.406 | 1.00 | 0.00 H | |
| ATOM | 882 | N | THR A | 65158.763 | 2.871 | 2.353 | 1.00 | 0.00 N | |

| ATOM | 883 | CA | THR A | 65159.400 | 3.850 | 1.481 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 884 | C | THR A | 65159.035 | 3.600 | 0.022 | 1.00 | 0.00 C |
| ATOM | 885 | О | THR A | 65159.312 | 2.531 | -0.524 | 1.00 | 0.00 O |
| ATOM | 886 | СВ | THR A | 65160.919 | 3.805 | 1.652 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.395 | 2.473 | 1.559 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.390 | 4.368 | 2.976 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.659 | 1.948 | 2.040 | 1.00 | 0.00 H |
| ATOM | 890 | НА | THR A | 65159.044 | 4.829 | 1.766 | 1.00 | 0.00 H |
| ATOM | 891 | НВ | THR A | 65161.377 | 4.385 | 0.865 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65161.050 | 2.065 | 0.762 | 1.00 | 0.00 H |
| ATOM | 893 | 1HG2 | THR A | 65160.959 | 5.348 | 3.123 | 1.00 | 0.00 H |
| ATOM | 894 | 2HG2 | THR A | 65162.466 | 4.445 | 2.972 | 1.00 | 0.00 H |
| ATOM | 895 | 3HG2 | THR A | 65161.078 | 3.714 | 3.777 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.411 | 4.591 | -0.606 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.008 | 4.479 | -2.003 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.094 | 5.022 | -2.927 | 1.00 | 0.00 C |
| ATOM | 899 | · O | PHE A | 66159.201 | 6.230 | -3.130 | 1.00 | 0.00 O |
| ATOM | 900 | CB | PHE A | 66156.697 | 5.230 | -2.241 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.012 | 4.848 | -3.522 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.529 | 5.822 | -4.381 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.849 | 3.516 | -3.865 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66154.899 | 5.474 | -5.560 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.218 | 3.161 | -5.042 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.742 | 4.141 | -5.892 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.218 | 5.419 | -0.118 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66157.857 | 3.432 | -2.220 | 1.00 | 0.00 H |
| ATOM | 909 | 1HB | PHE A | 66156.019 | 5.023 | -1.427 | 1.00 | 0.00 H |

| ATOM | 910 2 | 2НВ | PHE A | 66156.900 | 6.290 | -2.274 | 1.00 | 0.00 H |
|------|-------|-------|-------|-----------|---------|---------|------|--------|
| ATOM | 911 | HD1 | PHE A | 66155.652 | 6.864 | -4.124 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.220 | 2.748 | -3.202 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66154.528 | 6.242 | -6.223 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.098 | 2.119 | -5.299 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.250 | 3.867 | -6.812 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.896 | 4.119 | -3.483 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67160.973 | 4.509 | -4.386 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.960 | 5.438 | -3.686 | 1.00 | 0.00 C |
| ATOM | 919 | O | ARG A | 67162.592 | 6.281 | -4.322 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67160.404 | 5.194 | -5.629 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67159.247 | 4.438 | -6.263 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67158.335 | 5.371 | -7.047 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67158.608 | 5.327 | -8.481 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67158.258 | 4.314 | -9.271 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67157.622 | 3.261 | -8.771 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67158.544 | 4.354 - | -10.566 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.759 | 3.170 | -3.282 | 1.00 | 0.00 H |
| ATOM | 928 | HA | ARG A | 67161.493 | 3.612 | -4.686 | 1.00 | 0.00 H |
| ATOM | 929 1 | HB | ARG A | 67160.055 | 6.179 | -5.355 | 1.00 | 0.00 H |
| ATOM | 930 2 | 2HB | ARG A | 67161.188 | 5.290 | -6.365 | 1.00 | 0.00 H |
| ATOM | 931 1 | HG | ARG A | 67159.642 | 3.691 | -6.935 | 1.00 | 0.00 H |
| ATOM | 932 2 | 2HG | ARG A | 67158.673 | 3.959 | -5.484 | 1.00 | 0.00 H |
| ATOM | 933 1 | HD | ARG A | 67157.310 | 5.077 | -6.876 | 1.00 | 0.00 H |
| ATOM | 934 2 | 2HD | ARG A | 67158.483 | 6.380 | -6.691 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67159.077 | 6.091 | -8.876 | 1.00 | 0.00 H |
| ATOM | 936 1 | IHHI. | ARG A | 67157.403 | 3.225 | -7.795 | 1.00 | 0.00 H |

| ATOM | 937 2 | 2HH1 | ARG A | 67157.361 | 2.504 | -9.370 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 938 | HH2 | ARG A | 67159.022 | 5.145 - | 10.947 | 1.00 | 0.00 H |
| ATOM | 939 2 | 2HH2 | ARG A | 67158.282 | 3.594 - | 11.159 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.086 | 5.279 | -2.372 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68162.998 | 6.111 | -1.610 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.279 | 7.180 | -0.808 | 1.00 | 0.00 C |
| ATOM | 943 | О | GLY A | 68162.795 | 7.658 | 0.202 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68161.558 | 4.591 | -1.917 | 1.00 | 0.00 H |
| ATOM | 945 | lHA | GLY A | 68163.558 | 5.485 | -0.931 | 1.00 | 0.00 H |
| ATOM | 946 2 | 2HA | GLY A | 68163.686 | 6.590 | -2.291 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.086 | 7.556 | -1.260 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.299 | 8.575 | -0.576 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69159.624 | 8.002 | 0.666 | 1.00 | 0.00 C |
| ATOM | 950 | О | THR A | 69158.538 | 7.428 | 0.585 | 1.00 | 0.00 O |
| ATOM | 951 | СВ | THR A | 69159.245 | 9.152 | -1.523 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69159.760 | 9.271 | -2.836 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69158.746 | 10.518 | -1.101 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.728 | 7.138 | -2.070 | 1.00 | 0.00 H |
| ATOM | 955 | НА | THR A | 69160.969 | 9.365 | -0.275 | 1.00 | 0.00 H |
| ATOM | 956 | HB | THR A | 69158.396 | 8.484 | -1.549 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69159.603 | 8.454 | -3.317 | 1.00 | 0.00 H |
| ATOM | 958 | HG2 | THR A | 69157.684 | 10.586 | -1.285 | 1.00 | 0.00 H |
| ATOM | 959 2 | 2HG2 | THR A | 69159.259 | 11.280 | -1.670 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69158.939 | 10.663 | -0.048 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.275 | 8.161 | 1.813 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.738 | 7.659 | 3.073 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.513 | 8.463 | 3.499 | 1.00 | 0.00 C |

| ATOM | 964 | О | ARG A | 70158.554 | 9.692 | 3.554 | 1.00 | 0.00 O | |
|------|-------|------|-------|-----------|-------|-------|------|--------|--|
| ATOM | 965 | CB | ARG A | 70160.806 | 7.716 | 4.166 | 1.00 | 0.00 C | |
| ATOM | 966 | CG | ARG A | 70160.332 | 7.181 | 5.508 | 1.00 | 0.00 C | |
| ATOM | 967 | CD | ARG A | 70160.920 | 7.975 | 6.663 | 1.00 | 0.00 C | |
| ATOM | 968 | NE | ARG A | 70162.233 | 7.472 | 7.062 | 1.00 | 0.00 N | |
| ATOM | 969 | CZ | ARG A | 70163.084 | 8.150 | 7.828 | 1.00 | 0.00 C | |
| ATOM | 970 | NHI | ARG A | 70162.766 | 9.356 | 8.281 | 1.00 | 0.00 N | |
| ATOM | 971 | NH2 | ARG A | 70164.258 | 7.619 | 8.143 | 1.00 | 0.00 N | |
| ATOM | 972 | Н | ARG A | 70161.137 | 8.627 | 1.813 | 1.00 | 0.00 H | |
| ATOM | 973 | HA | ARG A | 70159.444 | 6.631 | 2.921 | 1.00 | 0.00 H | |
| ATOM | 974 1 | lНВ | ARG A | 70161.659 | 7.134 | 3.851 | 1.00 | 0.00 H | |
| ATOM | 975 2 | 2НВ | ARG A | 70161.112 | 8.743 | 4.300 | 1.00 | 0.00 H | |
| ATOM | 976 1 | IHG | ARG A | 70159.255 | 7.245 | 5.551 | 1.00 | 0.00 H | |
| ATOM | 977 2 | 2HG | ARG A | 70160.636 | 6.149 | 5.600 | 1.00 | 0.00 H | |
| ATOM | 978 1 | HD | ARG A | 70161.017 | 9.007 | 6.361 | 1.00 | 0.00 H | |
| ATOM | 979 2 | 2HD | ARG A | 70160.248 | 7.909 | 7.506 | 1.00 | 0.00 H | |
| ATOM | 980 | HE | ARG A | 70162.494 | 6.584 | 6.741 | 1.00 | 0.00 H | |
| ATOM | 981 1 | HH1 | ARG A | 70161.882 | 9.762 | 8.048 | 1.00 | 0.00 H | |
| ATOM | 982 2 | 2HH1 | ARG A | 70163.409 | 9.859 | 8.857 | 1.00 | 0.00 H | |
| ATOM | 983 1 | HH2 | ARG A | 70164.503 | 6.711 | 7.805 | 1.00 | 0.00 H | |
| ATOM | 984 2 | 2HH2 | ARG A | 70164.898 | 8.127 | 8.720 | 1.00 | 0.00 H | |
| ATOM | 985 | N | TYR A | 71157.426 | 7.760 | 3.799 | 1.00 | 0.00 N | |
| ATOM | 986 | CA | TYR A | 71156.189 | 8.408 | 4.220 | 1.00 | 0.00 C | |
| ATOM | 987 | C | TYR A | 71155.841 | 8.032 | 5.657 | 1.00 | 0.00 C | |
| ATOM | 988 | O | TYR A | 71155.425 | 8.880 | 6.447 | 1.00 | 0.00 O | |
| ATOM | 989 | CB | TYR A | 71155.042 | 8.019 | 3.287 | 1.00 | 0.00 C | |
| ATOM | 990 | CG | TYR A | 71155.198 | 8.551 | 1.879 | 1.00 | 0.00 C | |

| ATOM | 991 | CD1 | TYR A | 71155.353 | 7.686 | 0.804 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 992 | CD2 | TYR A | 71155.192 | 9.917 | 1.628 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.496 | 8.168 | -0.485 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.334 | 10.406 | 0.343 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.486 | 9.528 | -0.709 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71155.628 | 10.012 | -1.989 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.456 | 6.783 | 3.735 | 1.00 | 0.00 H |
| ATOM | 998 | НА | TYR A | 71156.339 | 9.476 | 4.167 | 1.00 | 0.00 H |
| ATOM | 999 | lНВ | TYR A | 71154.983 | 6.943 | 3.229 | 1.00 | 0.00 H |
| ATOM | 1000 2 | 2HB | TYR A | 71154.116 | 8.405 | 3.687 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.360 | 6.621 | 0.982 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.073 | 10.603 | 2.454 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.615 | 7.480 | -1.308 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.326 | 11.472 | 0.168 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71154.788 | 10.360 | -2.295 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72156.013 | 6.757 | 5.987 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.716 | 6.268 | 7.329 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.781 | 5.282 | 7.797 | 1.00 | 0.00 C |
| ATOM | 1009 | O | PHE A | 72157.740 | 5.001 | 7.079 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72154.339 | 5.603 | 7.358 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72154.122 | 4.623 | 6.241 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72154.270 | 3.261 | 6.457 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72153.771 | 5.062 | 4.974 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72154.071 | 2.357 | 5.431 | 1.00 | 0.00 C |
| ATOM | 1015 | CE2 | PHE A | 72153.570 | 4.163 | 3.944 | 1.00 | 0.00 C |
| ATOM | 1016 | CZ | PHE A | 72153.720 | 2.809 | 4.173 | 1.00 | 0.00 C |
| ATOM | 1017 | Н | PHE A | 72156.346 | 6.129 | 5.313 | 1.00 | 0.00 H |

| ATOM | 1018 | HA | PHE A | 72155.710 | 7.117 | 7.997 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1019 | 1HB | PHE A | 72154.223 | 5.072 | 8.291 | 1.00 | 0.00 H |
| ATOM | 1020 | 2HB | PHE A | 72153.578 | 6.365 | 7.285 | 1.00 | 0.00 H |
| ATOM | 1021 | HD1 | PHE A | 72154.543 | 2.908 | 7.440 | 1.00 | 0.00 H |
| ATOM | 1022 | HD2 | PHE A | 72153.653 | 6.120 | 4.795 | 1.00 | 0.00 H |
| ATOM | 1023 | HE1 | PHE A | 72154.190 | 1.300 | 5.612 | 1.00 | 0.00 H |
| ATOM | 1024 | HE2 | PHE A | 72153.297 | 4.519 | 2.962 | 1.00 | 0.00 H |
| ATOM | 1025 | HZ | PHE A | 72153.564 | 2.104 | 3.370 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73156.605 | 4.760 | 9.007 | 1.00 | 0.00 N |
| ATOM | 1027 | CA | THR A | 73157.551 | 3.805 | 9.573 | 1.00 | 0.00 C |
| ATOM | 1028 | C | THR A | 73156.871 | 2.469 | 9.856 | 1.00 | 0.00 C |
| ATOM | 1029 | О | THR A | 73156.113 | 2.338 | 10.817 | 1.00 | 0.00 O |
| ATOM | 1030 | CB | THR A | 73158.162 | 4.361 | 10.860 | 1.00 | 0.00 C |
| ATOM | 1031 | OG1 | THR A | 73157.244 | 5.211 | 11.525 | 1.00 | 0.00 O |
| ATOM | 1032 | CG2 | THR A | 73159.432 | 5.152 | 10.626 | 1.00 | 0.00 C |
| ATOM | 1033 | Н | THR A | 73155.821 | 5.023 | 9.533 | 1.00 | 0.00 H |
| ATOM | 1034 | HA | THR A | 73158.337 | 3.648 | 8.850 | 1.00 | 0.00 H |
| ATOM | 1035 | HB | THR A | 73158.401 | 3.539 | 11.518 | 1.00 | 0.00 H |
| ATOM | 1036 | HG1 | THR A | 73156.707 | 4.692 | 12.128 | 1.00 | 0.00 H |
| ATOM | 1037 | 1HG2 | THR A | 73159.457 | 5.998 | 11.296 | 1.00 | 0.00 H |
| ATOM | 1038 2 | 2HG2 | THR A | 73159.456 | 5.500 | 9.604 | 1.00 | 0.00 H |
| ATOM | 1039 | 3HG2 | THR A | 73160.288 | 4.521 | 10.812 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYSA | 74157.149 | 1.479 | 9.013 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74156.565 | 0.153 | 9.173 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74157.648 | -0.922 | 9.171 | 1.00 | 0.00 C |
| ATOM | 1043 | O . | CYSA | 74158.817 | -0.639 | 8.913 | 1.00 | 0.00 O |
| ATOM | 1044 | CB | CYS A | 74155.556 | -0.121 | 8.056 | 1.00 | 0.00 C |

| ATOM | 1045 | SG | CYS A | 74153.872 | 0.415 | 8.436 | 1.00 | 0.00 S |
|------|------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1046 | Н | CYS A | 74157.762 | 1.645 | 8.266 | 1.00 | 0.00 H |
| ATOM | 1047 | НА | CYS A | 74156.052 | 0.128 | 10.122 | 1.00 | 0.00 H |
| ATOM | 1048 | 1HB | CYS A | 74155.871 | 0.396 | 7.162 | 1.00 | 0.00 H |
| ATOM | 1049 | 2HB | CYS A | 74155.527 | -1.183 | 7.860 | 1.00 | 0.00 H |
| ATOM | 1050 | HG | CYS A | 74153.370 | -0.356 | 8.709 | 1.00 | 0.00 H |
| ATOM | 1051 | N | ALA A | 75157.249 | -2.157 | 9.460 | 1.00 | 0.00 N |
| ATOM | 1052 | CA | ALAA | 75158.185 | -3.274 | 9.491 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75158.860 | -3.461 | 8.137 | 1.00 | 0.00 C |
| ATOM | 1054 | O | ALA A | 75158.563 | -2.747 | 7.180 | 1.00 | 0.00 O |
| ATOM | 1055 | СВ | ALA A | 75157.469 | -4.549 | 9.908 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALA A | 75156.303 | -2.320 | 9.657 | 1.00 | 0.00 H |
| ATOM | 1057 | HA | ALA A | 75158.940 | -3.054 | 10.232 | 1.00 | 0.00 H |
| ATOM | 1058 | 1HB | ALA A | 75156.425 | -4.479 | 9.643 | 1.00 | 0.00 H |
| ATOM | 1059 | 2HB | ALA A | 75157.562 | -4.681 | 10.976 | 1.00 | 0.00 H |
| ATOM | 1060 | 3HB | ALA A | 75157.913 | -5.393 | 9.401 | 1.00 | 0.00 H |
| ATOM | 1061 | N | LEU A | 76159.770 | -4.427 | 8.064 | 1.00 | 0.00 N |
| ATOM | 1062 | CA | LEU A | 76160.488 | -4.709 | 6.827 | 1.00 | 0.00 C |
| ATOM | 1063 | C | LEU A | 76159.705 | -5.684 | 5.953 | 1.00 | 0.00 C |
| ATOM | 1064 | Ο | LEU A | 76159.141 | -6.660 | 6.447 | 1.00 | 0.00 O |
| ATOM | 1065 | CB | LEU A | 76161.873 | -5.281 | 7.135 | 1.00 | 0.00 C |
| ATOM | 1066 | CG | LEU A | 76162.966 | -4.238 | 7.375 | 1.00 | 0.00 C |
| ATOM | 1067 | CD1 | LEU A | 76164.095 | -4.830 | 8.205 | 1.00 | 0.00 C |
| ATOM | 1068 | CD2 | LEU A | 76163.495 | -3.708 | 6.051 | 1.00 | 0.00 C |
| ATOM | 1069 | Н | LEU A | 76159.964 | -4.963 | 8.862 | 1.00 | 0.00 H |
| ATOM | 1070 | HA | LEU A | 76160.604 | -3.778 | 6.292 | 1.00 | 0.00 H |
| ATOM | 1071 | 1HB | LEU A | 76161.795 | -5.901 | 8.016 | 1.00 | 0.00 H |

| ATOM | 1072 2 | HB | LEU A | 76162.176 | -5.901 | 6.305 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|-------|------|--------|
| ATOM | 1073 | HG | LEU A | 76162.547 | -3.408 | 7.926 | 1.00 | 0.00 H |
| ATOM | 1074 1 | HD1 | LEU A | 76164.504 | -4.068 | 8.851 | 1.00 | 0.00 H |
| ATOM | 1075 2 | HD1 | LEU A | 76164.869 | -5.199 | 7.548 | 1.00 | 0.00 H |
| ATOM | 1076 3 | HD1 | LEU A | 76163.713 | -5.643 | 8.803 | 1.00 | 0.00 H |
| ATOM | 1077 1 | HD2 | LEU A | 76163.973 | -2.752 | 6.212 | 1.00 | 0.00 H |
| ATOM | 1078 2 | HD2 | LEU A | 76162.676 | -3.589 | 5.357 | 1.00 | 0.00 H |
| ATOM | 1079 3 | HD2 | LEU A | 76164.213 | -4.406 | 5.645 | 1.00 | 0.00 H |
| ATOM | 1080 | N | LYS A | 77159.676 | -5.413 | 4.652 | 1.00 | 0.00 N |
| ATOM | 1081 | CA | LYS A | 77158.962 | -6.266 | 3.709 | 1.00 | 0.00 C |
| ATOM | 1082 | C | LYS A | 77157.473 | -6.313 | 4.036 | 1.00 | 0.00 C |
| ATOM | 1083 | Ο | LYS A | 77156.840 | -7.365 | 3.949 | 1.00 | 0.00 O |
| ATOM | 1084 | CB | LYS A | 77159.546 | -7.681 | 3.727 | 1.00 | 0.00 C |
| ATOM | 1085 | CG | LYS A | 77161.022 | -7.735 | 3.366 | 1.00 | 0.00 C |
| ATOM | 1086 | CD | LYS A | 77161.222 | -7.948 | 1.874 | 1.00 | 0.00 C |
| ATOM | 1087 | CE | LYS A | 77162.466 | -7.232 | 1.372 | 1.00 | 0.00 C |
| ATOM | 1088 | NZ | LYS A | 77163.176 | -8.018 | 0.325 | 1.00 | 0.00 N |
| ATOM | 1089 | Н | LYS A | 77160.145 | -4.620 | 4.319 | 1.00 | 0.00 H |
| ATOM | 1090 | HA | LYS A | 77159.089 | -5.848 | 2.722 | 1.00 | 0.00 H |
| ATOM | 1091 1 | HB | LYS A | 77159.425 | -8.095 | 4.717 | 1.00 | 0.00 H |
| ATOM | 1092 2 | HB | LYS A | 77159.002 | -8.292 | 3.022 | 1.00 | 0.00 H |
| ATOM | 1093 1 | HG | LYS A | 77161.487 | -6.804 | 3.653 | 1.00 | 0.00 H |
| ATOM | 1094 2 | HG | LYS A | 77161.484 | -8.552 | 3.902 | 1.00 | 0.00 H |
| ATOM | 1095 1 | HD | LYS A | 77161.325 | -9.005 | 1.681 | 1.00 | 0.00 H |
| ATOM | 1096 2 | HD | LYS A | 77160.360 | -7.566 | 1.347 | 1.00 | 0.00 H |
| ATOM | 1097 1 | HE | LYSA | 77162.174 | -6.278 | 0.956 | 1.00 | 0.00 H |
| ATOM | 1098 2 | HE | LYS A | 77163.133 | -7.070 | 2.205 | 1.00 | 0.00 H |

| ATOM | 1099 1 | HZ | LYS A | 77162.881 | -7.702 | -0.620 / | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|----------|------|--------|
| ATOM | 1100 2 | 2HZ | LYS A | 77162.953 | -9.029 | 0.426 | 1.00 | 0.00 H |
| ATOM | 1101 3 | BHZ | LYS A | 77164.204 | -7.890 | 0.418 | 1.00 | 0.00 H |
| ATOM | 1102 | N | LYS A | 78156.919 | - 5.165 | 4.412 | 1.00 | 0.00 N |
| ATOM | 1103 | CA | LYS A | 78155.503 | -5.075 | 4.751 | 1.00 | 0.00 C |
| ATOM | 1104 | C | LYS A | 78154.937 | -3.711 | 4.366 | 1.00 | 0.00 C |
| ATOM | 1105 | О | LYS A | 78154.084 | -3.163 | 5.064 | 1.00 | 0.00 O |
| ATOM | 1106 | СВ | LYS A | 78155.299 | -5.322 | 6.246 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.835 | -6.663 | 6.719 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78155.588 | -6.870 | 8.205 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYSA | 78154.371 | -7.748 | 8.450 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYSA | 78153.592 | -7.299 | 9.636 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.475 | -4.359 | 4.462 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.980 | -5.838 | 4.193 | 1.00 | 0.00 H |
| ATOM | 1113 1 | НВ | LYS A | 78155.801 | -4.543 | 6.800 | 1.00 | 0.00 H |
| ATOM | 1114 2 | HB | LYS A | 78154.242 | -5.284 | 6.464 | 1.00 | 0.00 H |
| ATOM | 1115 1 | HG | LYS A | 78155.342 | -7.451 | 6.169 | 1.00 | 0.00 H |
| ATOM | 1116 2 | HG | LYS A | 78156.898 | -6.702 | 6.531 | 1.00 | 0.00 H |
| ATOM | 1117 1 | HD | LYS A | 78156.454 | -7.342 | 8.641 | 1.00 | 0.00 H |
| ATOM | 1118 2 | HD | LYS A | 78155.426 | -5.908 | 8.669 | 1.00 | 0.00 H |
| ATOM | 1119 1 | HE | LYS A | 78153.736 | -7.712 | 7.578 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYS A | 78154.703 | -8.764 | 8.611 | 1.00 | 0.00 H |
| ATOM | 1121 1 | HZ | LYS A | 78154.204 | -6.763 | 10.284 | 1.00 | 0.00 H |
| ATOM | 1122 2 | 2HZ | LYS A | 78153.207 | -8.121 | 10.144 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYSA | 78152.803 | -6.691 | 9.336 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.417 | -3.170 | 3.252 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.959 | -1.871 | 2.774 | 1.00 | 0.00 C |

| ATOM | 1126 | C | ALA A | 79154.768 | -1.878 | 1.261 | 1.00 | 0.00 C |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1127 | О | ALA A | 79155.729 | -1.743 | 0.504 | 1.00 | 0.00 O |
| ATOM | 1128 | CB | ALA A | 79155.942 | -0.784 | 3.179 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79156.096 | -3.655 | 2.738 | 1.00 | 0.00 H |
| ATOM | 1130 | HA | ALA A | 79154.010 | -1.659 | 3.246 | 1.00 | 0.00 H |
| ATOM | 1131 | 1HB | ALA A | 79155.400 | 0.113 | 3.442 | 1.00 | 0.00 H |
| ATOM | 1132 2 | 2HB | ALA A | 79156.607 | -0.573 | 2.354 | 1.00 | 0.00 H |
| ATOM | 1133 3 | ЗНВ | ALA A | 79156.519 | -1.117 | 4.028 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.522 | -2.038 | 0.829 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.204 | -2.063 | -0.595 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.375 | -0.846 | -0.989 | 1.00 | 0.00 C |
| ATOM | 1137 | O | LEU A | 80151.319 | -0.587 | -0.410 | 1.00 | 0.00 O |
| ATOM | 1138 | CB | LEU A | 80152.448 | -3.345 | -0.947 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.015 | -3.461 | -2.409 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.127 | -4.072 | -3.247 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80150.742 | -4.287 | -2.524 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.798 | -2.140 | 1.481 | 1.00 | 0.00 H |
| ATOM | 1143 | HA | LEU A | 80154.135 | -2.042 | -1.143 | 1.00 | 0.00 H |
| ATOM | 1144 | 1HB | LEU A | 80153.083 | -4.188 | -0.712 | 1.00 | 0.00 H |
| ATOM | 1145 | 2HB | LEU A | 80151.565 | -3.399 | -0.328 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.811 | -2.473 | -2.795 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | LEU A | 80153.127 | -3.621 | -4.229 | 1.00 | 0.00 H |
| ATOM | 11482 | 2HD1 | LEU A | 80152.964 | -5.136 | -3.340 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80154.078 | -3.894 | -2.769 | 1.00 | 0.00 H |
| ATOM | 1150 | 1HD2 | LEU A | 80150.387 | -4.261 | -3.543 | 1.00 | 0.00 H |
| ATOM | 1151 2 | 2HD2 | LEU A | 80149.988 | -3.878 | -1.868 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80150.950 | -5.308 | -2.240 | 1.00 | 0.00 H |

| ATOM | 1153 | N | PHE A | 81152.859 | -0.100 | -1.976 | 1.00 | 0.00 N |
|------|------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1154 | CA | PHE A | 81152.162 | 1.091 | -2.449 | 1:00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.323 | 0.776 | -3.683 | 1.00 | 0.00 C |
| ATOM | 1156 | О | PHE A | 81151.796 | 0.136 | -4.621 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.164 | 2.201 | -2.768 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.781 | 2.823 | -1.548 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81154.882 | 2.242 | -0.940 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81153.260 | 3.988 | -1.009 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81155.453 | 2.812 | 0.182 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81153.826 | 4.563 | 0.113 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81154.924 | 3.973 | 0.710 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.705 | -0.357 | -2.399 | 1.00 | 0.00 H |
| ATOM | 1165 | HA | PHE A | 81151.507 | 1.426 | -1.658 | 1.00 | 0.00 H |
| ATOM | 1166 | 1HB | PHE A | 81153.961 | 1.794 | -3.372 | 1.00 | 0.00 H |
| ATOM | 1167 | 2HB | PHE A | 81152.662 | 2.981 | -3.323 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81155.297 | 1.334 | -1.352 | 1.00 | 0.00 H |
| ATOM | 1169 | HD2 | PHE A | 81152.401 | 4.449 | -1.475 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81156.311 | 2.349 | 0.646 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81153.410 | 5.471 | 0.523 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.368 | 4.421 | 1.586 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.074 | 1.230 | -3.674 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VALA | 82149.168 | 0.997 | -4.793 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VAL A | 82148.207 | 2.167 | -4.975 | 1.00 | 0.00 C |
| ATOM | 1176 | Ο | VAL A | 82148.090 | 3.029 | -4.105 | 1.00 | 0.00 O |
| ATOM | 1177 | CB | VALA | 82148.354 | -0.295 | -4.597 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VAL A | 82149.264 | -1.512 | -4.631 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VAL A | 82147.570 | -0.241 | -3.294 | 1.00 | 0.00 C |

| ATOM | 1180 | Н | VAL A | 82149.753 | 1.734 | -2.896 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1181 | НА | VAL A | 82149.764 | 0.890 | -5.687 | 1.00 | 0.00 H |
| ATOM | 1182 | HB | VAL A | 82147.648 | -0.379 | -5.412 | 1.00 | 0.00 H |
| ATOM | 1183 | 1HG1 | VAL A | 82150.134 | -1.294 | -5.233 | 1.00 | 0.00 H |
| ATOM | 1184 | 2HG1 | VAL A | 82148.732 | -2.349 | -5.058 | 1.00 | 0.00 H |
| ATOM | 1185 | 3HG1 | VAL A | 82149.574 | -1.758 | -3.626 | 1.00 | 0.00 H |
| ATOM | 1186 | 1HG2 | VAL A | 82147.581 | -1.214 | -2.825 | 1.00 | 0.00 H |
| ATOM | 1187 | 2HG2 | VAL A | 82146.551 | 0.050 | -3.498 | 1.00 | 0.00 H |
| ATOM | 1188 | 3HG2 | VAL A | 82148.025 | 0.482 | -2.631 | 1.00 | 0.00 H |
| ATOM | 1189 | N | LYS A | 83147.522 | 2.190 | -6.114 | 1.00 | 0.00 N |
| ATOM | 1190 | CA | LYS A | 83146.571 | 3.255 | -6.413 | 1.00 | 0.00 C |
| ATOM | 1191 | C | LYS A | 83145.380 | 3.204 | -5.464 | 1.00 | 0.00 C |
| ATOM | 1192 | O | LYS A | 83144.707 | 2.180 | -5.348 | 1.00 | 0.00 O |
| ATOM | 1193 | CB | LYS A | 83146.091 | 3.145 | -7.860 | 1.00 | 0.00 C |
| ATOM | 1194 | CG | LYS A | 83147.213 | 3.230 | -8.882 | 1.00 | 0.00 C |
| ATOM | 1195 | CD | LYS A | 83146.736 | 2.827 | -10.268 | 1.00 | 0.00 C |
| ATOM | 1196 | CE | LYS A | 83147.304 | 3.741 | -11.341 | 1.00 | 0.00 C |
| ATOM | 1197 | NZ | LYS A | 83147.522 | 3.022 | -12.627 | 1.00 | 0.00 N |
| ATOM | 1198 | Н | LYS A | 83147.660 | 1.475 | -6.769 | 1.00 | 0.00 H |
| ATOM | 1199 | HA | LYS A | 83147.079 | 4.199 | -6.281 | 1.00 | 0.00 H |
| ATOM | 1200 | 1HB | LYS A | 83145.586 | 2.200 | -7.989 | 1.00 | 0.00 H |
| ATOM | 1201 | 2HB | LYS A | 83145.393 | 3.945 | -8.058 | 1.00 | 0.00 H |
| ATOM | 1202 | 1HG | LYS A | 83147.577 | 4.246 | -8.918 | 1.00 | 0.00 H |
| ATOM | 1203 | 2HG | LYS A | 83148.012 | 2.569 | -8.579 | 1.00 | 0.00 H |
| ATOM | 1204 | 1HD | LYS A | 83147.055 | 1.814 | -10.467 | 1.00 | 0.00 H |
| ATOM | 1205 | 2HD | LYS A | 83145.658 | 2.878 | -10.297 | 1.00 | 0.00 H |
| ATOM | 1206 | 1HE | LYSA | 83146.613 | 4.554 - | 11.507 | 1.00 | 0.00 H |

| ATOM | 1207 2HE | LYS A | 83148.247 | 4.137 - | 10.995 | 1.00 | 0.00 H |
|------|-----------|---------|-----------|---------|---------|------|--------|
| ATOM | 1208 1HZ | LYS A | 83148.420 | 2.497 - | 12.595 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83147.557 | 3.699 - | 13.414 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83146.746 | 2.349 - | 12.796 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.125 | 4.318 | -4.788 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.015 | 4.410 | -3.849 | 1.00 | 0.00 C |
| ATOM | 1213 C | LEU A | 84142.685 | 4.149 | -4.549 | 1.00 | 0.00 C |
| ATOM | 1214 O | LEU A | 84141.743 | 3.636 | -3.944 | 1.00 | 0.00 O |
| ATOM | 1215 CB | LEU A | 84143.997 | 5.791 | -3.189 | 1.00 | 0.00 C |
| ATOM | 1216 CG | LEU A | 84142.811 | 6.051 | -2.258 | 1.00 | 0.00 C |
| ATOM | 1217 CD | I LEU A | 84142.917 | 5.194 | -1.006 | 1.00 | 0.00 C |
| ATOM | 1218 CD2 | 2 LEU A | 84142.737 | 7.526 | -1.891 | 1.00 | 0.00 C |
| ATOM | 1219 H | LEU A | 84145.698 | 5.101 | -4.926 | 1.00 | 0.00 H |
| ATOM | 1220 HA | LEU A | 84144.162 | 3.659 | -3.087 | 1.00 | 0.00 H |
| ATOM | 1221 1HB | LEU A | 84144.908 | 5.907 | -2.620 | 1.00 | 0.00 H |
| ATOM | 1222 2HB | LEU A | 84143.984 | 6.537 | -3.969 | 1.00 | 0.00 H |
| ATOM | 1223 HG | LEU A | 84141.896 | 5.786 | -2.767 | 1.00 | 0.00 H |
| ATOM | 1224 1HD1 | LEU A | 84143.435 | 5.745 | -0.236 | 1.00 | 0.00 H |
| ATOM | 1225 2HD1 | LEU A | 84143.465 | 4.291 | -1.234 | 1.00 | 0.00 H |
| ATOM | 1226 3HD1 | LEU A | 84141.927 | 4.936 | - 0.662 | 1.00 | 0.00 H |
| ATOM | 1227 1HD2 | LEUA | 84141.795 | 7.729 | -1.404 | 1.00 | 0.00 H |
| ATOM | 1228 2HD2 | LEUA | 84142.815 | 8.124 | -2.787 | 1.00 | 0.00 H |
| ATOM | 1229 3HD2 | LEUA | 84143.549 | 7.772 | -1.222 | 1.00 | 0.00 H |
| ATOM | 1230 N | LYSA | 85142.616 | 4.505 | -5.827 | 1.00 | 0.00 N |
| ATOM | 1231 CA | LYS A | 85141.401 | 4.310 | -6.611 | 1.00 | 0.00 C |
| ATOM | 1232 C | LYS A | 85141.072 | 2.826 | -6.754 | 1.00 | 0.00 C |
| ATOM | 1233 O | LYS A | 85139.912 | 2.453 | -6.932 | 1.00 | 0.00 O |

| ATOM | 1234 CB | LYS A | 85141.555 | 4.944 | -7.994 | 1.00 | 0.00 C |
|------|----------|-------|-----------|----------|--------|------|--------|
| ATOM | 1235 CG | LYS A | 85142.656 | 4.315 | -8.833 | 1.00 | 0.00 C |
| ATOM | 1236 CD | LYS A | 85143.327 | 5.341 | -9.732 | 1.00 | 0.00 C |
| ATOM | 1237 CE | LYS A | 85142.637 | 5.432 - | 11.083 | 1.00 | 0.00 C |
| ATOM | 1238 NZ | LYS A | 85141.191 | 5.755 - | 10.950 | 1.00 | 0.00 N |
| ATOM | 1239 H | LYS A | 85143.400 | 4.910 | -6.254 | 1.00 | 0.00 H |
| ATOM | 1240 HA | LYS A | 85140.590 | 4.797 | -6.091 | 1.00 | 0.00 H |
| ATOM | 1241 1HB | LYS A | 85140.622 | 4.844 | -8.529 | 1.00 | 0.00 H |
| ATOM | 1242 2HB | LYS A | 85141,779 | 5.994 | -7.874 | 1.00 | 0.00 H |
| ATOM | 1243 1HG | LYS A | 85143.397 | 3.888 | -8.175 | 1.00 | 0.00 H |
| ATOM | 1244 2HG | LYS A | 85142.226 | 3.537 | -9.447 | 1.00 | 0.00 H |
| ATOM | 1245 1HD | LYS A | 85143.284 | 6.308 | -9.252 | 1.00 | 0.00 H |
| ATOM | 1246 2HD | LYS A | 85144.358 | 5.055 | -9.881 | 1.00 | 0.00 H |
| ATOM | 1247 1HE | LYS A | 85143.117 | 6.205 -1 | 1.666 | 1.00 | 0.00 H |
| ATOM | 1248 2HE | LYS A | 85142.741 | 4.484 -1 | 1.590 | 1.00 | 0.00 H |
| ATOM | 1249 1HZ | LYS A | 85140.781 | 5.957 -1 | 1.884 | 1.00 | 0.00 H |
| ATOM | 1250 2HZ | LYS A | 85141.065 | 6.590 -1 | 0.342 | 1.00 | 0.00 H |
| ATOM | 1251 3HZ | LYS A | 85140.683 | 4.953 -1 | 0.526 | 1.00 | 0.00 H |
| ATOM | 1252 N | SER A | 86142.098 | 1.984 | -6.674 | 1.00 | 0.00 N |
| ATOM | 1253 CA | SER A | 86141.913 | 0.542 | -6.794 | 1.00 | 0.00 C |
| ATOM | 1254 C | SER A | 86141.835 | -0.115 | -5.420 | 1.00 | 0.00 C |
| ATOM | 1255 O | SER A | 86142.239 | -1.265 | -5.247 | 1.00 | 0.00 O |
| ATOM | 1256 CB | SER A | 86143.057 | -0.073 | -7.602 | 1.00 | 0.00 C |
| ATOM | 1257 OG | SER A | 86143.348 | 0.704 | -8.751 | 1.00 | 0.00 O |
| ATOM | 1258 H | SER A | 86143.000 | 2.340 | -6.531 | 1.00 | 0.00 H |
| ATOM | 1259 HA | SER A | 86140.984 | 0.370 | -7.316 | 1.00 | 0.00 H |
| ATOM | 1260 1HB | SER A | 86143.942 | -0.126 | -6.986 | 1.00 | 0.00 H |

| ATOM | 1261 2 | 2HB | SER A | 86142.778 | -1.068 | -7.916 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1262 | HG | SER A | 86144.296 | 0.706 | -8.905 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.311 | 0.621 | -4.445 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.180 | 0.107 | -3.086 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87139.712 | 0.006 | -2.683 | 1.00 | 0.00 C |
| ATOM | 1266 | О | CYS A | 87138.868 | 0.749 | -3.182 | 1.00 | 0.00 O |
| ATOM | 1267 | СВ | CYS A | 87141.929 | 1.008 | -2.104 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYS A | 87143.720 | 1.039 | -2.349 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYS A | 87141.005 | 1.530 | -4.642 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87141.616 | -0.880 | -3.061 | 1.00 | 0.00 H |
| ATOM | 1271 1 | IНВ | CYS A | 87141.568 | 2.020 | -2.207 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.741 | 0.665 | -1.096 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.138 | 0.829 | -1.511 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.416 | -0.921 | -1.777 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.050 | -1.121 | -1.307 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.005 | -1.203 | 0.219 | 1.00 | 0.00 C |
| ATOM | 1277 | O | ARG A | 88138.924 | -1.729 | 0.846 | 1.00 | 0.00 O |
| ATOM | 1278 | CB | ARG A | 88137.458 | -2.394 | -1.918 | 1.00 | 0.00 C |
| ATOM | .1279 | CG | ARG A | 88136.431 | -2.125 | -3.009 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.076 | -2.726 | -2.667 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88134.097 | -1.701 | -2.312 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88133.646 | -0.781 | -3.162 | 1.00 | 0.00 C |
| ATOM | 1283 | NH1 | ARG A | 88134.084 | -0.752 | -4.414 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88132.754 | 0.114 | -2.758 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.132 | -1.484 | -1.416 | 1.00 | 0.00 H |
| ATOM | 1286 | HA | ARG A | 88137.463 | -0.273 | -1.627 | 1.00 | 0.00 H |
| ATOM | 1287 | lНВ | ARG A | 88138.260 | -2.978 | -2.346 | 1.00 | 0.00 H |

| ATOM | 1288 | 2HB | ARG A | 88136.983 | -2.969 | -1.138 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1289 | 1HG | ARG A | 88136.320 | -1.057 | -3.128 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88136.784 | -2.557 | -3.934 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88134.714 | -3.274 | -3.524 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.195 | -3.401 | -1.832 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88133.756 | -1.699 | -1.393 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88134.757 | -1.424 | -4.726 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88133.742 | -0.058 | -5.047 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88132.420 | 0.097 | -1.815 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88132.416 | 0.806 | -3.395 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89136.930 | -0.683 | 0.838 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89136.774 | -0.703 | 2.296 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89136.931 | -2.105 | 2.875 | 1.00 | 0.00 C |
| ATOM | 1301 | О | PRO A | 89136.144 | -3.003 | 2.574 | 1.00 | 0.00 O |
| ATOM | 1302 | СВ | PRO A | 89135.347 | -0.195 | 2.512 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.044 | 0.615 | 1.300 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89135.786 | -0.038 | 0.168 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.475 | -0.037 | 2.777 | 1.00 | 0.00 H |
| ATOM | 1306 | 1HB | PRO A | 89134.675 | -1.035 | 2.605 | 1.00 | 0.00 H |
| ATOM | 1307 | 2HB | PRO A | 89135.308 | 0.406 | 3.408 | 1.00 | 0.00 H |
| ATOM | 1308 | 1HG | PRO A | 89133.981 | 0.605 | 1.108 | 1.00 | 0.00 H |
| ATOM | 1309 | 2HG | PRO A | 89135.391 | 1.628 | 1.439 | 1.00 | 0.00 H |
| ATOM | 1310 | 1HD | PRO A | 89135.160 | -0.772 | -0.319 | 1.00 | 0.00 H |
| ATOM | 1311 | 2HD | PRO A | 89136.122 | 0.703 | -0.541 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASP A | 90137.951 | -2.286 | 3.707 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASP A | 90138.210 | -3.579 | 4.329 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.750 | -3.586 | 5.783 | 1.00 | 0.00 C |

| ATOM | 1315 | Ο | ASPA | 90138.340 | -2.918 | 6.633 | 1.00 | 0.00 O |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1316 | CB | ASP A | 90139.699 | -3.915 | 4.251 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90139.952 | -5.409 | 4.179 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASPA | 90140.458 | -5.974 | 5.171 | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | ASPA | 90139.643 | -6.013 | 3.131 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.543 | -1.532 | 3.909 | 1.00 | 0.00 H |
| ATOM | 1321 | HA | ASPA | 90137.652 | -4.326 | 3.784 | 1.00 | 0.00 H |
| ATOM | 1322 | HB | ASP A | 90140.121 | -3.455 | 3.370 | 1.00 | 0.00 H |
| ATOM | 1323 2 | 2HB | ASPA | 90140.195 | -3.527 | 5.128 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.697 | -4.345 | 6.063 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91136.163 | -4.439 | 7.417 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91136.405 | -5.826 | 8.004 | 1.00 | 0.00 C |
| ATOM | 1327 | O | SER A | 91135.654 | -6.286 | 8.864 | 1.00 | 0.00 O |
| ATOM | 1328 | CB | SER A | 91134.664 | -4.130 | 7.419 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91134.264 | -3.549 | 8.648 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91136.270 | -4.856 | 5.344 | 1.00 | 0.00 H |
| ATOM | 1331 | НА | SER A | 91136.672 | -3.708 | 8.027 | 1.00 | 0.00 H |
| ATOM | 1332 | lНВ | SER A | 91134.440 | -3.440 | 6.619 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91134.111 | -5.046 | 7.272 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91134.508 | -2.620 | 8.658 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92137.459 | -6.487 | 7.536 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92137.799 | -7.821 | 8.017 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92138.193 | -7.782 | 9.490 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92137.991 | -8.751 | 10.223 | 1.00 | 0.00 O |
| ATOM | 1339 | CB | ARG A | 92138.940 | -8.410 | 7.187 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92138.468 | -9.193 | 5.972 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92138.300 | -8.294 | 4.757 | 1.00 | 0.00 C |

| ATOM | 1342 | NE | ARG A | 92136.945 | -8.354 | 4.214 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 1343 | CZ | ARG A | 92136.620 | -7.964 | 2.984 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92137.549 | -7.484 | 2.165 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92135.364 | -8.053 | 2.569 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92138.021 | -6.068 | 6.851 | 1.00 | 0.00 H |
| ATOM | 1347 | HA | ARG A | 92136.925 | -8.445 | 7.907 | 1.00 | 0.00 H |
| ATOM | 1348 | 1HB | ARG A | 92139.575 | -7.605 | 6.845 | 1.00 | 0.00 H |
| ATOM | 1349 | 2HB | ARG A | 92139.520 | -9.073 | 7.812 | 1.00 | 0.00 H |
| ATOM | 1350 | 1HG | ARG A | 92139.195 | -9.958 | 5.744 | 1.00 | 0.00 H |
| ATOM | 1351 | 2HG | ARG A | 92137.518 | -9.654 | 6.201 | 1.00 | 0.00 H |
| ATOM | 1352 | 1HD | ARG A | 92138.517 | -7.276 | 5.043 | 1.00 | 0.00 H |
| ATOM | 1353 | 2HD | ARG A | 92138.997 | -8.609 | 3.994 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92136.240 | -8.704 | 4.798 | 1.00 | 0.00 H |
| ATOM | 1355 | 1HH1 | ARG A | 92138.499 | -7.414 | 2.472 | 1.00 | 0.00 H |
| ATOM | 1356 | 2HH1 | ARG A | 92137.299 | -7.193 | 1.242 | 1.00 | 0.00 H |
| ATOM | 1357 | 1HH2 | ARG A | 92134.660 | -8.414 | 3.182 | 1.00 | 0.00 H |
| ATOM | 1358 | 2HH2 | ARG A | 92135.120 | - 7.759 | 1.646 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93138.757 | -6.657 | 9.917 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93139.180 | -6.492 | 11.304 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93138.401 | -5.369 | 11.982 | 1.00 | 0.00 C |
| ATOM | 1362 | О | PHE A | 93138.910 | -4.705 | 12.885 | 1.00 | 0.00 O |
| ATOM | 1363 | CB | PHE A | 93140.679 | -6.198 | 11.369 | 1.00 | 0.00 Ç |
| ATOM | 1364 | CG | PHE A | 93141.523 | -7.226 | 10.669 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93142.351 | -8.069 | 11.393 | 1.00 | 0.00 C |
| ATOM | .1366 | CD2 | PHE A | 93141.487 | -7.347 | 9.290 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93143.128 | -9.015 | 10.752 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93142.262 | -8.291 | 8.643 | 1.00 | 0.00 C |

| ATOM | 1369 | CZ | PHE A | 93143.084 | -9.127 | 9.375 | 1.00 | 0.00 C | |
|------|--------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 1370 | Н | PHE A | 93138.892 | -5.919 | 9.286 | 1.00 | 0.00 H | |
| ATOM | 1371 | HA | PHE A | 93138.980 | -7.417 | 11.823 | 1.00 | 0.00 H | |
| ATOM | 1372 1 | НВ | PHE A | 93140.872 | -5.241 | 10.908 | 1.00 | 0.00 H | |
| ATOM | 1373 2 | 2HB | PHE A | 93140.986 | -6.162 | 12.404 | 1.00 | 0.00 H | |
| ATOM | 1374 | HD1 | PHE A | 93142.386 | -7.983 | 12.469 | 1.00 | 0.00 H | |
| ATOM | 1375 | HD2 | PHE A | 93140.845 | -6.695 | 8.717 | 1.00 | 0.00 H | |
| ATOM | 1376 | HE1 | PHE A | 93143.770 | -9.667 | 11.326 | 1.00 | 0.00 H | |
| ATOM | 1377 | HE2 | PHE A | 93142.225 | -8.376 | 7.567 | 1.00 | 0.00 H | |
| ATOM | 1378 | HZ | PHE A | 93143.690 | -9.865 | 8.873 | 1.00 | 0.00 H | |
| ATOM | 1379 | N | ALA A | 94137.162 | -5.162 | 11.543 | 1.00 | 0.00 N | |
| ATOM | 1380 | CA | ALAA | 94136.315 | -4.119 | 12.109 | 1.00 | 0.00 C | |
| ATOM | 1381 | C | ALAA | 94136.137 | -4.315 | 13.612 | 1.00 | 0.00 C | |
| ATOM | 1382 | O | ALAA | 94135.661 | -5.358 | 14.061 | 1.00 | 0.00 O | |
| ATOM | 1383 | CB | ALA A | 94134.964 | -4.101 | 11.410 | 1.00 | 0.00 C | |
| ATOM | 1384 | Н | ALA A | 94136.811 | -5.723 | 10.819 | 1.00 | 0.00 H | |
| ATOM | 1385 | HA | ALA A | 94136.796 | -3.168 | 11.936 | 1.00 | 0.00 H | |
| ATOM | 1386 1 | НВ | ALA A | 94134.900 | -3.232 | 10.773 | 1.00 | 0.00 H | |
| ATOM | 1387 2 | HB | ALA A | 94134.175 | -4.065 | 12.147 | 1.00 | 0.00 H | |
| ATOM | 1388 3 | НВ | ALA A | 94134.856 | -4.994 | 10.812 | 1.00 | 0.00 H | |
| ATOM | 1389 | N | SER A | 95136.521 | -3.304 | 14.385 | 1.00 | 0.00 N | |
| ATOM | 1390 | CA | SER A | 95136.403 | -3.364 | 15.837 | 1.00 | 0.00 C | |
| ATOM | 1391 | C | SER A | 95134.940 | -3.417 | 16.263 | 1.00 | 0.00 C | |
| ATOM | 1392 | O | SER A | 95134.056 | -2.942 | 15.549 | 1.00 | 0.00 O | |
| ATOM | 1393 | CB | SER A | 95137.088 | -2.155 | 16.476 | 1.00 | 0.00 C | |
| ATOM | 1394 | OG | SER A | 95138.479 | -2.154 | 16.204 | 1.00 | 0.00 O | |
| ATOM | 1395 | Н | SER A | 95136.892 | -2.498 | 13.968 | 1.00 | 0.00 H | |

| ATOM | 1396 | НА | SER A | 95136.895 | -4.265 | 16.172 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1397 | 1HB | SER A | 95136.657 | -1.249 | 16.081 | 1.00 | 0.00 H |
| ATOM | 1398 | 2HB | SER A | 95136.943 | -2.187 | 17.546 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95138.947 | -2.573 | 16.930 | 1.00 | 0.00 H |
| ATOM | 1400 | N | LEU A | 96134.689 | -3.999 | 17.432 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96133.333 | -4.114 | 17.954 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96132.453 | -4.926 | 17.010 | 1.00 | 0.00 C |
| ATOM | 1403 | О | LEU A | 96131.929 | -4.402 | 16.027 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96132.727 | -2.726 | 18.167 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96131.527 | -2.680 | 19.115 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96131.490 | -1.359 | 19.866 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96130.232 | -2.895 | 18.344 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96135.436 | -4.359 | 17.956 | 1.00 | 0.00 H |
| ATOM | 1409 | ,HA | LEU A | 96133.386 | -4.624 | 18.904 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96133.496 | -2.077 | 18.561 | 1.00 | 0.00 H |
| ATOM | 1411 | 2HB | LEU A | 96132.413 | -2.342 | 17.208 | 1.00 | 0.00 H |
| ATOM | 1412 | HG | LEU A | 96131.621 | -3.475 | 19.840 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96131.103 | -0.587 | 19.218 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96132.487 | -1.097 | 20.183 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96130.851 | -1.456 | 20.732 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96130.444 | -3.422 | 17.426 | 1.00 | 0.00 H |
| ATOM | 1417 | 2HD2 | LEU A | 96129.787 | -1.938 | 18.116 | 1.00 | 0.00 H |
| ATOM | 1418 | 3HD2 | LEU A | 96129.548 | -3.477 | 18.945 | 1.00 | 0.00 H |
| ATOM | 1419 | N | GLN A | 97132.295 | -6.211 | 17.314 | 1.00 | 0.00 N |
| ATOM | 1420 | CA | GLN A | 97131.478 | -7.096 | 16.492 | 1.00 | 0.00 C |
| ATOM | 1421 | C | GLN A | 97130.853 | -8.204 | 17.339 | 1.00 | 0.00 C |
| ATOM | 1422 | O | GLN A | 97131.005 | -9.388 | 17.040 | 1.00 | 0.00 O |

| ATOM | 1423 | CB | GLN A | 97132.321 | -7.708 | 15.371 | 1.00 | 0.00 C |
|------|--------|------|-------|-------------|---------|--------|------|--------|
| ATOM | 1424 | CG | GLN A | 97131.511 | -8.109 | 14.149 | 1.00 | 0.00 C |
| ATOM | 1425 | CD | GLN A | 97132.049 | -9.356 | 13.476 | 1.00 | 0.00 C |
| ATOM | 1426 | OE1 | GLN A | 97132.386 - | -10.337 | 14.138 | 1.00 | 0.00 O |
| ATOM | 1427 | NE2 | GLN A | 97132.134 | -9.323 | 12.151 | 1.00 | 0.00 N |
| ATOM | 1428 | Н | GLN A | 97132.738 | -6.571 | 18.110 | 1.00 | 0.00 H |
| ATOM | 1429 | HA | GLN A | 97130.687 | -6.506 | 16.055 | 1.00 | 0.00 H |
| ATOM | 1430 | 1HB | GLN A | 97133.065 | -6.987 | 15.061 | 1.00 | 0.00 H |
| ATOM | 1431 2 | 2HB | GLN A | 97132.821 | -8.588 | 15.750 | 1.00 | 0.00 H |
| ATOM | 1432 | HG | GLN A | 97130.492 | -8.296 | 14.455 | 1.00 | 0.00 H |
| ATOM | 1433 2 | 2HG | GLN A | 97131.530 | -7.296 | 13.438 | 1.00 | 0.00 H |
| ATOM | 1434 | HE2 | GLN A | 97131.847 | -8.508 | 11.689 | 1.00 | 0.00 H |
| ATOM | 1435 2 | 2HE2 | GLN A | 97132.478 - | 10.116 | 11.690 | 1.00 | 0.00 H |
| ATOM | 1436 | N | PRO A | 98130.137 | -7.830 | 18.413 | 1.00 | 0.00 N |
| ATOM | 1437 | CA | PRO A | 98129.487 | -8.797 | 19.305 | 1.00 | 0.00 C |
| ATOM | 1438 | C | PRO A | 98128.279 | -9.461 | 18.655 | 1.00 | 0.00 C |
| ATOM | 1439 | O | PRO A | 98128.061 | -9.336 | 17.449 | 1.00 | 0.00 O |
| ATOM | 1440 | CB | PRO A | 98129.050 | -7.941 | 20.495 | 1.00 | 0.00 C |
| ATOM | 1441 | CG | PRO A | 98128.876 | -6.573 | 19.933 | 1.00 | 0.00 C |
| ATOM | 1442 | CD | PRO A | 98129.904 | -6.437 | 18.843 | 1.00 | 0.00 C |
| ATOM | 1443 | HA | PRO A | 98130.179 | -9.556 | 19.637 | 1.00 | 0.00 H |
| ATOM | 1444 | 1HB | PRO A | 98128.126 | -8.326 | 20.898 | 1.00 | 0.00 H |
| ATOM | 1445 | 2HB | PRO A | 98129.817 | -7.960 | 21.256 | 1.00 | 0.00 H |
| ATOM | 1446 | 1HG | PRO A | 98127.881 | -6.469 | 19.526 | 1.00 | 0.00 H |
| ATOM | 1447 | 2HG | PRO A | 98129.046 | -5.836 | 20.703 | 1.00 | 0.00 H |
| ATOM | 1448 | 1HD | PRO A | 98129.515 | -5.843 | 18.029 | 1.00 | 0.00 H |
| ATOM | 1449 | 2HD | PRO A | 98130.810 | -5.998 | 19.233 | 1.00 | 0.00 H |

| ATOM | 1450 | N | SER A | 99127.494 -10.169 | 19.462 | 1.00 | 0.00 N | |
|--------|--------|-----|---------|--------------------|--------|------|--------|--|
| ATOM | 1451 | CA | SER A | 99126.306 -10.854 | 18.966 | 1.00 | 0.00 C | |
| ATOM | 1452 | C | SER A | 99125.385 -11.247 | 20.115 | 1.00 | 0.00 C | |
| ATOM | 1453 | О | SER A | 99125.840 -11.743 | 21.146 | 1.00 | 0.00 O | |
| ATOM | 1454 | СВ | SER A | 99126.704 -12.096 | 18.168 | 1.00 | 0.00 C | |
| ATOM | 1455 | OG | SER A | 99127.637 -11.774 | 17.150 | 1.00 | 0.00 O | |
| ATOM | 1456 | Н | SER A | 99127.719 -10.231 | 20.413 | 1.00 | 0.00 H | |
| ATOM | 1457 | НА | SER A | 99125.778 -10.172 | 18.315 | 1.00 | 0.00 H | |
| ATOM | 1458 | lНВ | SER A | 99127.153 -12.820 | 18.832 | 1.00 | 0.00 H | |
| ATOM | 1459 2 | 2HB | SER A | 99125.824 -12.526 | 17.710 | 1.00 | 0.00 H | |
| ATOM | 1460 | HG | SER A | 99128.438 -12.286 | 17.275 | 1.00 | 0.00 H | |
| ATOM | 1461 | N | GLY A | 100124.088 -11.024 | 19.932 | 1.00 | 0.00 N | |
| ATOM | 1462 | CA | GLY A | 100123.124 -11.361 | 20.963 | 1.00 | 0.00 C | |
| ATOM | 1463 | C | GLY A 1 | 100121.706 -11.447 | 20.429 | 1.00 | 0.00 C | |
| ATOM | 1464 | O | GLY A | 100120.983 -10.451 | 20.420 | 1.00 | 0.00 O | |
| ATOM | 1465 | Н | GLY A | 100123.782 -10.626 | 19.090 | 1.00 | 0.00 H | |
| ATOM | 1466 | lHA | GLY A 1 | 100123.394 -12.314 | 21.393 | 1.00 | 0.00 H | |
| ATOM | 1467 2 | 2HA | GLY A | 100123.161 -10.607 | 21.736 | 1.00 | 0.00 H | |
| ATOM | 1468 | N | PRO A | 101121.277 -12.635 | 19.970 | 1.00 | 0.00 N | |
| ATOM | 1469 | CA | PRO A | 101119.927 -12.833 | 19.431 | 1.00 | 0.00 C | |
| ATOM | 1470 | C | PRO A | 101118.856 -12.759 | 20.514 | 1.00 | 0.00 C | |
| ATOM | 1471 | O | PRO A | 101117.797 -12.164 | 20.313 | 1.00 | 0.00 O | |
| ATOM . | 1472 | СВ | PRO A | 101119.986 -14.239 | 18.833 | 1.00 | 0.00 C | |
| ATOM | 1473 | CG | PRO A | 101121.058 -14.933 | 19.599 | 1.00 | 0.00 C | |
| ATOM | 1474 | CD | PRO A | 101122.072 -13.877 | 19.941 | 1.00 | 0.00 C | |
| ATOM | 1475 | НА | PRO A | 101119.703 -12.117 | 18.655 | 1.00 | 0.00 H | |
| ATOM | 1476 | 1HB | PRO A | 101119.030 -14.727 | 18.958 | 1.00 | 0.00 H | |

| ATOM | 1477 2 | 2HB | PRO A 101120.230 -14.177 | 17.782 | 1.00 | 0.00 H |
|------|--------|-----|--------------------------|--------|------|--------|
| ATOM | 1478 | IHG | PRO A 101120.646 -15.363 | 20.501 | 1.00 | 0.00 H |
| ATOM | 1479 2 | 2HG | PRO A 101121.508 -15.702 | 18.989 | 1.00 | 0.00 H |
| ATOM | 1480 | IHD | PRO A 101122.513 -14.076 | 20.907 | 1.00 | 0.00 H |
| ATOM | 1481 2 | 2HD | PRO A 101122.836 -13.827 | 19.179 | 1.00 | 0.00 H |
| ATOM | 1482 | N | SER A 102119.138 -13.367 | 21.661 | 1.00 | 0.00 N |
| ATOM | 1483 | CA | SER A 102118.198 -13.369 | 22.776 | 1.00 | 0.00 C |
| ATOM | 1484 | C | SER A 102116.891 -14.051 | 22.386 | 1.00 | 0.00 C |
| ATOM | 1485 | О | SER A 102116.548 -14.126 | 21.206 | 1.00 | 0.00 O |
| ATOM | 1486 | СВ | SER A 102117.922 -11.938 | 23.242 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102118.809 -11.557 | 24.277 | 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102119.999 -13.824 | 21.760 | 1.00 | 0.00 H |
| ATOM | 1489 | HA | SER A 102118.650 -13.921 | 23.588 | 1.00 | 0.00 H |
| ATOM | 1490 | lНВ | SER A 102118.047 -11.261 | 22.410 | 1.00 | 0.00 H |
| ATOM | 1491 2 | 2НВ | SER A 102116.908 -11.872 | 23.609 | 1.00 | 0.00 H |
| ATOM | 1492 | HG | SER A 102119.210 -10.712 | 24.061 | 1.00 | 0.00 H |
| ATOM | 1493 | N | SER A 103116.168 -14.548 | 23.383 | 1.00 | 0.00 N |
| ATOM | 1494 | CA | SER A 103114.898 -15.225 | 23.144 | 1.00 | 0.00 C |
| ATOM | 1495 | C | SER A 103113.728 -14.368 | 23.617 | 1.00 | 0.00 C |
| ATOM | 1496 | O | SER A 103113.660 -13.981 | 24.784 | 1.00 | 0.00 O |
| ATOM | 1497 | CB | SER A 103114.875 -16.578 | 23.856 | 1.00 | 0.00 C |
| ATOM | 1498 | OG | SER A 103115.624 -16.535 | 25.059 | 1.00 | 0.00 O |
| ATOM | 1499 | Н | SER A 103116.495 -14.458 | 24.303 | 1.00 | 0.00 H |
| ATOM | 1500 | HA | SER A 103114.804 -15.386 | 22.081 | 1.00 | 0.00 H |
| ATOM | 1501 | lНВ | SER A 103113.855 -16.840 | 24.093 | 1.00 | 0.00 H |
| ATOM | 1502 2 | 2HB | SER A 103115.299 -17.330 | 23.208 | 1.00 | 0.00 H |
| ATOM | 1503 | HG | SER A 103116.371 -17.133 | 24.992 | 1.00 | 0.00 H |

GLY A 104112.809 -14.076 22.702 1.00 0.00 N **ATOM** 1504 N CA GLY A 104111.653 -13.267 23.046 1.00 0.00 C **ATOM** 1505 GLY A 104112.037 -11.875 23.512 1.00 0.00 C **ATOM** 1506 С GLY A 104111.578 -11.468 24.600 1.00 0.00 O **ATOM** 1507 O **ATOM** 1508 OXT GLY A 104112.796 -11.196 22.791 1.00 0.00 O 1509 H GLY A 104112.915 -14.411 21.788 0.00 H**ATOM** 1.00 **ATOM** 1510 1HA GLY A 104111.018 -13.179 22.176 1.00 0.00 H**ATOM** 1511 2HA GLY A 104111.103 -13.760 23.833 1.00 0.00 H 1512 GLY A 104 TER **ENDMDL**

Three-Dimensional Structure Coordinate Table 5

ATOM 1 N GLY A 1119.934 2.882 -11.176 1.00 0.00 C ATOM 2 CA GLY A 1120.718 4.087 -11.473 1.00 0.00 C ATOM 3 C GLY A 1121.589 ATOM 4 O GLY A 1122.802 4.050 -11.266 1.00 0.00 O ATOM 5 1H GLY A 1120.404 1.634 -12.822 1.00 0.00 H 3.217 -13.049 1.00 0.00 H ATOM 6 2H GLY A 1119.854 ATOM 7 3H GLY A 1118.978 2.151 -12.071 1.00 0.00 H 3.135 -10.380 1.00 0.00 H ATOM 8 1HA GLY A 1120.034 2.067 -10.851 1.00 0.00 H ATOM 9 2HA GLY A 1121.348 2120.970 5.157 -11.960 1.00 0.00 N ATOM10 N SER A 2121.698 6.378 -12.287 1.00 0.00 C ATOM11 CA SER A 2122.748 6.115 -13.362 1.00 0.00 C ATOM12 C SER A 2123.937 6.005 -13.067 1.00 0.00 O ATOM13 O SER A 6.950 -11.035 1.00 0.00 C ATOM14 CB SER A 2122.364 ATOM15 OG SER A 2121.480 7.806 -10.331 1.00 0.00 O

| ATOM16 | Н | SER A | 2120.001 | 5.125 -12.104 | 1.00 | 0.00 H |
|----------|-----|-------|----------|---------------|------|--------|
| ATOM17 | НА | SER A | 2120.985 | 7.096 -12.665 | 1.00 | 0.00 H |
| ATOM18 1 | НВ | SER A | 2122.654 | 6.140 -10.382 | 1.00 | 0.00 H |
| ATOM19 2 | 2HB | SER A | 2123.239 | 7.514 -11.321 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2121.576 | 7.661 -9.387 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3122.299 | 6.016 -14.609 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3123.200 | 5.765 -15.728 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3123.931 | 4.438 -15.551 | 1.00 | 0.00 C |
| ATOM24 | О | SER A | 3123.690 | 3.708 -14.590 | 1.00 | 0.00 O |
| ATOM25 | СВ | SER A | 3124.211 | 6.905 -15.859 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3123.566 | 8.124 -16.188 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3121.339 | 6.112 -14.781 | 1.00 | 0.00 H |
| ATOM28 | НА | SER A | 3122.605 | 5.717 -16.628 | 1.00 | 0.00 H |
| ATOM29 1 | НВ | SER A | 3124.734 | 7.030 -14.923 | 1.00 | 0.00 H |
| ATOM30 2 | 2HB | SER A | 3124.919 | 6.666 -16.639 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3122.788 | 8.233 -15.637 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4124.827 | 4.134 -16.485 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4125.580 | 2.896 -16.413 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4126.815 | 3.017 -15.541 | 1.00 | 0.00 C |
| ATOM35 | O | GLY A | 4127.021 | 4.037 -14.883 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4124.978 | 4.755 -17.227 | 1.00 | 0.00 H |
| ATOM37 1 | HA | GLY A | 4124.942 | 2.122 -16.011 | 1.00 | 0.00 H |
| ATOM38 2 | 2HA | GLY A | 4125.883 | 2.614 -17.411 | 1.00 | 0.00 H |
| АТОМ39 | N | SER A | 5127.638 | 1.973 -15.537 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5128.859 | 1.967 -14.740 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5128.541 | 2.115 -13.255 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5127.375 | 2.182 -12.864 | 1.00 | 0.00 O |

| ATOM43 | CB | SER A | 5129.792 | 3.093 -1 | 15.188 | 1.00 | 0.00 C |
|----------|-----|-------|----------|----------|--------|------|--------|
| ATOM44 | OG | SER A | 5130.310 | 2.842 - | 16.482 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5127.419 | 1.190 -1 | 6.083 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5129.352 | 1.019 - | 14.897 | 1.00 | 0.00 H |
| ATOM47 | НВ | SER A | 5129.245 | 4.025 -1 | 5.208 | 1.00 | 0.00 H |
| ATOM48 2 | 2HB | SER A | 5130.615 | 3.174 -1 | 4.493 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5130.634 | 1.939 - | 16.528 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6129.584 | 2.166 -1 | 2.434 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6129.415 | 2.307 -1 | 10.992 | 1.00 | 0.00 C |
| ATOM52 | С | SER A | 6128.918 | 3.704 -1 | 0.637 | 1.00 | 0.00 C |
| ATOM53 | О | SER A | 6128.643 | 4.519 -1 | 1.517 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6130.735 | 2.024 -1 | 10.273 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6130.834 | 0.658 | -9.907 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6130.488 | 2.108 -1 | 2.805 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6128.680 | 1.584 - | 10.673 | 1.00 | 0.00 H |
| ATOM58 | ΙНВ | SER A | 6131.558 | 2.268 -1 | 0.928 | 1.00 | 0.00 H |
| ATOM59 2 | ΣНВ | SER A | 6130.794 | 2.629 | -9.380 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6131.760 | 0.409 | -9.847 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7128.805 | 3.974 | -9.340 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7128.341 | 5.274 | -8.891 | 1.00 | 0.00 C |
| ATOM63 | С | GLY A | 7129.005 | 5.713 | -7.601 | 1.00 | 0.00 C |
| ATOM64 | О | GLY A | 7129.918 | 5.051 | -7.108 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7129.039 | 3.285 | -8.683 | 1.00 | 0.00 H |
| ATOM66 | lHA | GLY A | 7128.552 | 6.003 | -9.658 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7127.273 | 5.228 | -8.736 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8128.544 | 6.833 | -7.053 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8129.099 | 7.360 | -5.811 | 1.00 | 0.00 C |

| ATOM70 C | LEU A | 8127.992 | 7.667 | -4.808 | 1.00 | 0.00 C |
|-------------|-------|----------|--------|--------|------|--------|
| ATOM71 O | LEU A | 8126.829 | 7.822 | -5.180 | 1.00 | 0.00 O |
| ATOM72 CB | LEU A | 8129.916 | 8.624 | -6.089 | 1.00 | 0.00 C |
| ATOM73 CG | LEU A | 8131.353 | 8.378 | -6.550 | 1.00 | 0.00 C |
| ATOM74 CD1 | LEU A | 8131.955 | 9.650 | -7.124 | 1.00 | 0.00 C |
| ATOM75 CD2 | LEUA | 8132.199 | 7.859 | -5.397 | 1.00 | 0.00 C |
| ATOM76 H | LEU A | 8127.814 | 7.315 | -7.493 | 1.00 | 0.00 H |
| ATOM77 HA | LEU A | 8129.750 | 6.607 | -5.392 | 1.00 | 0.00 H |
| ATOM78 1HB | LEU A | 8129.407 | 9.194 | -6.854 | 1.00 | 0.00 H |
| ATOM79 2HB | LEU A | 8129.947 | 9.213 | -5.186 | 1.00 | 0.00 H |
| ATOM80 HG | LEU A | 8131.352 | 7.628 | -7.328 | 1.00 | 0.00 H |
| ATOM81 1HD1 | LEU A | 8131.820 | 10.461 | -6.423 | 1.00 | 0.00 H |
| ATOM82 2HD1 | LEU A | 8131.462 | 9.894 | -8.054 | 1.00 | 0.00 H |
| ATOM83 3HD1 | LEU A | 8133.010 | 9.501 | -7.304 | 1.00 | 0.00 H |
| ATOM84 1HD2 | LEU A | 8132.928 | 7.157 | -5.772 | 1.00 | 0.00 H |
| ATOM85 2HD2 | LEU A | 8131.562 | 7.367 | -4.676 | 1.00 | 0.00 H |
| ATOM86 3HD2 | LEU A | 8132.706 | 8.686 | -4.922 | 1.00 | 0.00 H |
| ATOM87 N | ALA A | 9128.361 | 7.754 | -3.534 | 1.00 | 0.00 N |
| ATOM88 CA | ALA A | 9127.398 | 8.042 | -2.478 | 1.00 | 0.00 C |
| ATOM89 C | ALA A | 9128.053 | 8.796 | -1.326 | 1.00 | 0.00 C |
| ATOM90 O | ALA A | 9127.633 | 8.677 | -0.176 | 1.00 | 0.00 O |
| ATOM91 CB | ALAA | 9126.766 | 6.754 | -1.975 | 1.00 | 0.00 C |
| ATOM92 H | ALA A | 9129.303 | 7.619 | -3.299 | 1.00 | 0.00 H |
| АТОМ93 НА | ALA A | 9126.617 | 8.658 | -2.899 | 1.00 | 0.00 H |
| ATOM94 1HB | ALA A | 9127.284 | 6.421 | -1.087 | 1.00 | 0.00 H |
| ATOM95 2HB | ALA A | 9126.839 | 5.994 | -2.740 | 1.00 | 0.00 H |
| ATOM96 3HB | ALA'A | 9125.726 | 6.929 | -1.742 | 1.00 | 0.00 H |

| ATOM97 | N | МЕТ | `A 1012 | 9.085 9.5 | 73 -1.64 | 1.00 | 0.00 | N |
|--------|-------|-----|---------|-------------|----------|---------|------|--------|
| ATOM98 | CA | MET | A 1012 | 29.796 10.3 | 347 -0.6 | 33 1.00 | 0.00 | C |
| ATOM99 | C | MET | A 1013 | 0.666 11.4 | 22 -1.28 | 32 1.00 | 0.00 | С |
| ATOM | 100 | О | MET A | 10131.871 | 11.241 | -1.449 | 1.00 | 0.00 O |
| ATOM | 101 | СВ | MET A | 10130.664 | 9.427 | 0.230 | 1.00 | 0.00 C |
| ATOM | 102 | CG | MET A | 10130.012 | 9.038 | 1.548 | 1.00 | 0.00 C |
| ATOM | 103 | SD | MET A | 10130.760 | 9.864 | 2.965 | 1.00 | 0.00 S |
| ATOM | 104 | CE | MET A | 10132.424 | 9.208 | 2.903 | 1.00 | 0.00 C |
| ATOM | 105 | Н | MET A | 10129.373 | 9.628 | -2.578 | 1.00 | 0.00 H |
| ATOM | 106 | НА | MET A | 10129.061 | 10.827 | -0.005 | 1.00 | 0.00 H |
| ATOM | 107 | 1HB | MET A | 10130.870 | 8.525 | -0.325 | 1.00 | 0.00 H |
| ATOM | 108 2 | 2HB | MET A | 10131.596 | 9.928 | 0.446 | 1.00 | 0.00 H |
| ATOM | 109 | 1HG | MET A | 10128.966 | 9.301 | 1.508 | 1.00 | 0.00 H |
| ATOM | 110 2 | 2HG | MET A | 10130.109 | 7.970 | 1.680 | 1.00 | 0.00 H |
| ATOM | 111 1 | HE | MET A | 10132.732 | 9.103 | 1.872 | 1.00 | 0.00 H |
| ATOM | 112.2 | 2HE | MET A | 10132.449 | 8.242 | 3.384 | 1.00 | 0.00 H |
| ĄTOM | 113 3 | BHE | MET A | 10133.098 | 9.881 | 3.412 | 1.00 | 0.00 H |
| ATOM | 114 | N | PRO A | 11130.060 | 12.563 | -1.655 | 1.00 | 0.00 N |
| ATOM | 115 | CA | PRO A | 11130.787 | 13.668 | -2.285 | 1.00 | 0.00 C |
| ATOM | 116 | C | PRO A | 11131.997 | 14.110 | -1.464 | 1.00 | 0.00 C |
| ATOM | 117 | O | PRO A | 11133.081 | 14.317 | -2.011 | 1.00 | 0.00 O |
| ATOM | 118 | CB | PRO A | 11129.751 | 14.793 | -2.359 | 1.00 | 0.00 C |
| ATOM | 119 | CG | PRO A | 11128.428 | 14.110 | -2.301 | 1.00 | 0.00 C |
| ATOM · | 120 | CD | PRO A | 11128.627 | 12.861 | -1.489 | 1.00 | 0.00 C |
| ATOM | 121 | HA | PRO A | 11131.110 | 13.409 | -3.282 | 1.00 | 0.00 H |
| ATOM | 122 | 1HB | PRO A | 11129.886 | 15.465 | -1.524 | 1.00 | 0.00 H |
| ATOM | 123 | 2HB | PRO A | 11129.873 | 15.335 | -3.285 | 1.00 | 0.00 H |

| ATOM | 124 1HG | PRO A | 11127.708 | 14.752 | -1.821 | 1.00 | 0.00 H |
|------|---------|-------|-----------|--------|---------|------|--------|
| ATOM | 125 2HG | PRO A | 11128.101 | 13.859 | -3.300 | 1.00 | 0.00 H |
| ATOM | 126 1HD | PRO A | 11128.392 | 13.045 | -0.451 | 1.00 | 0.00 H |
| ATOM | 127 2HD | PRO A | 11128.020 | 12.057 | -1.877 | 1.00 | 0.00 H |
| ATOM | 128 N | PRO A | 12131.836 | 14.258 | -0.134 | 1.00 | 0.00 N |
| ATOM | 129 CA | PRO A | 12132.932 | 14.672 | 0.747 | 1.00 | 0.00 C |
| ATOM | 130 C | PRO A | 12134.071 | 13.659 | 0.754 | 1.00 | 0.00 C |
| ATOM | 131 O | PRO A | 12135.204 | 13.984 | 1.107 | 1.00 | 0.00 O |
| ATOM | 132 CB | PRO A | 12132.283 | 14.754 | 2.136 | 1.00 | 0.00 C |
| ATOM | 133 CG | PRO A | 12130.815 | 14.809 | 1.879 | 1.00 | 0.00 C |
| ATOM | 134 CD | PRO A | 12130.591 | 14.030 | 0.616 | 1.00 | 0.00 C |
| ATOM | 135 HA | PRO A | 12133.318 | 15.642 | 0.469 | 1.00 | 0.00 H |
| ATOM | 136 1HB | PRO A | 12132.549 | 13.879 | 2.711 | 1.00 | 0.00 H |
| ATOM | 137 2HB | PRO A | 12132.626 | 15.641 | 2.644 | 1.00 | 0.00 H |
| ATOM | 138 1HG | PRO A | 12130.281 | 14.354 | 2.700 | 1.00 | 0.00 H |
| ATOM | 139 2HG | PRO A | 12130.502 | 15.834 | 1.748 | 1.00 | 0.00 H |
| ATOM | 140 1HD | PRO A | 12130.458 | 12.981 | 0.837 | 1.00 | 0.00 H |
| ATOM | 141 2HD | PRO A | 12129.738 | 14.416 | 0.081 | 1.00 | 0.00 H |
| ATOM | 142 N | GLY A | 13133.759 | 12.427 | 0.361 | 1.00 | 0.00 N |
| ATOM | 143 CA | GLY A | 13134.766 | 11.384 | 0.327 | 1.00 | 0.00 C |
| ATOM | 144 C | GLY A | 13135.229 | 11.068 | - 1.082 | 1.00 | 0.00 C |
| ATOM | 145 O | GLY A | 13134.684 | 11.593 | -2.053 | 1.00 | 0.00 O |
| ATOM | 146 H | GLY A | 13132.837 | 12.226 | 0.090 | 1.00 | 0.00 H |
| ATOM | 147 1HA | GLY A | 13135.617 | 11.700 | 0.911 | 1.00 | 0.00 H |
| ATOM | 148 2HA | GLY A | 13134.355 | 10.487 | 0.768 | 1.00 | 0.00 H |
| ATOM | 149 N | ASN A | 14136.236 | 10.209 | -1.194 | 1.00 | 0.00 N |
| ATOM | 150 CA | ASN A | 14136.770 | 9.824 | -2.495 | 1.00 | 0.00 C |

| ATOM | 151 | C | ASN A | 14135.847 | 8.829 | -3.190 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 152 | О | ASN A | 14135.407 | 9.058 | -4.316 | 1.00 | 0.00 O |
| ATOM | 153 | CB | ASN A | 14138.167 | 9.219 | -2.337 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14139.066 | 10.061 | -1.454 | 1.00 | 0.00 C |
| ATOM | 155 | OD1 | ASN A | 14139.732 | 10.984 | -1.925 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14139.090 | 9.749 | -0.164 | 1.00 | 0.00 N |
| ATOM | 157 | Н | ASN A | 14136.629 | 9.823 | -0.383 | 1.00 | 0.00 H |
| ATOM | 158 | НА | ASN A | 14136.841 | 10.715 | -3.100 | 1.00 | 0.00 H |
| ATOM | 159 | IНВ | ASN A | 14138.079 | 8.237 | -1.896 | 1.00 | 0.00 H |
| ATOM | 160 2 | 2HB | ASN A | 14138.627 | 9.133 | -3.310 | 1.00 | 0.00 H |
| ATOM | 161 | HD2 | ASN A | 14138.535 | 9.002 | 0.142 | 1.00 | 0.00 H |
| ATOM | 162 2 | 2HD2 | ASN A | 14139.663 | 10.277 | 0.430 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15135.560 | 7.722 | -2.512 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15134.689 | 6.693 | -3.065 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15133.686 | 6.210 | -2.022 | 1.00 | 0.00 C |
| ATOM | 166 | О | SER A | 15132.492 | 6.099 | -2.300 | 1.00 | 0.00 O |
| ATOM | 167 | СВ | SER A | 15135.520 | 5.512 | -3.574 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15134.733 | 4.638 | -4.365 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15135.942 | 7.596 | -1.618 | 1.00 | 0.00 H |
| ATOM | 170 | НА | SER A | 15134.149 | 7.125 | -3.893 | 1.00 | 0.00 H |
| ATOM | 171 | IНВ | SER A | 15136.337 | 5.884 | -4.175 | 1.00 | 0.00 H |
| ATOM | 172 2 | 2HB | SER A | 15135.913 | 4.962 | -2.732 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15133.932 | 4.410 | -3.889 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16134.179 | 5.924 | -0.822 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.325 | 5.452 | 0.263 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16133.925 | 5.807 | 1.620 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.233 | 6.314 | 2.502 | 1.00 | 0.00 O |

| ATOM | 178 | CB | HIS A | 16133.124 | 3.940 | 0.160 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 179 | CG | HIS A | 16131.734 | 3.497 | 0.497 | 1.00 | 0.00 C |
| ATOM | 180 | NDI | HIS A | 16131.293 | 3.324 | 1.793 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16130.683 | 3.192 | -0.300 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16130.032 | 2.931 | 1.777 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16129.638 | 2.843 | 0.520 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16135.140 | 6.032 | -0.662 | 1.00 | 0.00 H |
| ATOM | 185 | НА | HIS A | 16132.367 | 5.942 | 0.166 | 1.00 | 0.00 H |
| ATOM | 186 | IHB | HIS A | 16133.337 | 3.623 | -0.849 | 1.00 | 0.00 H |
| ATOM | 187 2 | 2HB | HIS A | 16133.806 | 3.445 | 0.838 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16131.825 | 3.467 | 2.603 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16130.670 | 3.217 | -1.381 | 1.00 | 0.00 H |
| ATOM | 190 | HEI | HIS A | 16129.425 | 2.718 | 2.646 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16128.774 | 2.491 | 0.222 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.217 | 5.537 | 1.779 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17135.887 | 5.834 | 3.032 | 1.00 | 0.00 C |
| ATOM | .194 | C | GLY A | 17137.270 | 5.217 | 3.109 | 1.00 | 0.00 C |
| ATOM | 195 | O | GLY A | 17137.577 | 4.481 | 4.045 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.718 | 5.132 | 1.041 | 1.00 | 0.00 H |
| ATOM | 197 | IHA | GLY A | 17135.976 | 6.905 | 3.134 | 1.00 | 0.00 H |
| ATOM | 198 2 | 2HA | GLY A | 17135.289 | 5.453 | 3.846 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18138.106 | 5.519 | 2.121 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.464 | 4.989 | 2.080 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.482 | 6.077 | 2.411 | 1.00 | 0.00 C |
| ATOM | 202 | O | LEU A | 18140.788 | 6.929 | 1.578 | 1.00 | 0.00 O |
| ATOM | 203 | CB | LEU A | 18139.763 | 4.398 | 0.701 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18139.023 | 3.098 | 0.381 | 1.00 | 0.00 C |

| ATOM | 205 | CD1 | LEU A | 18138.916 | 2.902 | -1.124 | 1.00 | 0.00 C |
|-------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 206 | CD2 | LEU A | 18139.726 | 1.914 | 1.027 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.802 | 6.112 | 1.403 | 1.00 | 0.00 H |
| ATOM | 208 | НА | LEU A | 18139.537 | 4.207 | 2.821 | 1.00 | 0.00 H |
| ATOM | 209 | 1HB | LEU A | 18139.500 | 5.133 | -0.046 | 1.00 | 0.00 H |
| ATOM | 210 | 2HB | LEU A | 18140.824 | 4.207 | 0.636 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18138.021 | 3.154 | 0.781 | 1.00 | 0.00 H |
| ATOM | 212 | 1HD1 | LEU A | 18138.964 | 1.848 | -1.354 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18139.732 | 3.415 | -1.612 | 1.00 | 0.00 H |
| ATOM | 214 | 3HD1 | LEU A | 18137.978 | 3.305 | -1.473 | 1.00 | 0.00 H |
| ATOM | 215 | 1HD2 | LEU A | 18139.773 | 2.062 | 2.095 | 1.00 | 0.00 H |
| ATOM | 216 | 2HD2 | LEU A | 18140.726 | 1.828 | 0.630 | 1.00 | 0.00 H |
| ATOM | 217 | 3HD2 | LEU A | 18139.175 | 1.009 | 0.813 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19141.003 | 6.039 | 3.633 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.987 | 7.021 | 4.076 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19143.003 | 6.385 | 5.019 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19142.915 | 5.198 | 5.333 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19141.291 | 8.193 | 4.771 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.354 | 7.767 | 5.889 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19139.186 | 8.717 | 6.064 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19138.168 | 8.543 | 5.361 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19139.287 | 9.634 | 6.905 | 1.00 | 0.00 O |
| 'ATOM | 227 | Н | GLU A | 19140.719 | 5.335 | 4.253 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.504 | 7.388 | 3.202 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19142.043 | 8.845 | 5.190 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19140.717 | 8.741 | 4.040 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.968 | 6.784 | 5.664 | 1.00 | 0.00 H |

| ATOM | 232 | 2HG | GLU A | 19140.911 | 7.730 | 6.814 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|-------|-------|------|--------|
| ATOM | 233 | N | VAL A | 20143.968 | 7.183 | 5.466 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL A | 20145.001 | 6.699 | 6.374 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.390 | 6.120 | 7.646 | 1.00 | 0.00 C |
| ATOM | 236 | О | VALA | 20143.480 | 6.706 | 8.230 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20145.985 | 7.822 | 6.754 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20147.147 | 7.267 | 7.563 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VALA | 20146.487 | 8.537 | 5.508 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.984 | 8.120 | 5.180 | 1.00 | 0.00 H |
| ATOM | 241 | HA | VAL A | 20145.554 | 5.922 | 5.865 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.460 | 8.540 | 7.368 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20147.999 | 7.923 | 7.468 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20147.406 | 6.286 | 7.194 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20146.861 | 7.195 | 8.602 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20146.440 | 7.864 | 4.665 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20147.508 | 8.853 | 5.661 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20145.868 | 9.401 | 5.315 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.897 | 4.967 | 8.068 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.389 | 4.329 | 9.267 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.329 | 3.289 | 8.967 | 1.00 | 0.00 C |
| ATOM | 252 | Ο | GLY A | 21143.299 | 2.225 | 9.586 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.624 | 4.546 | 7.561 | 1.00 | 0.00 H |
| ATOM | 254 | 1HA | GLY A | 21145.208 | 3.852 | 9.784 | 1.00 | 0.00 H |
| ATOM | 255 | 2HA | GLY A | 21143.963 | 5.084 | 9.912 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.455 | 3.595 | 8.013 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.387 | 2.679 | 7.631 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.933 | 1.524 | 6.796 | 1.00 | 0.00 C |

| ATOM | 259 | О | SER A | 22142.942 | 1.668 | 6.106 | 1.00 | 0.00 O |
|--------|-----|------|-------|-----------|---------|--------|------|--------|
| ATOM | 260 | СВ | SER A | 22140.304 | 3.423 | 6.847 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22140.042 | 4.693 | 7.418 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.530 | 4.459 | 7.555 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22140.953 | 2.280 | 8.535 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.632 | 3.561 | 5.828 | 1.00 | 0.00 H |
| ATOM | 265 | 2HB | SER A | 22139.393 | 2.842 | 6.856 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22139.251 | 5.065 | 7.021 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.259 | 0.381 | 6.865 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.677 | -0.798 | 6.116 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.131 | -0.761 | 4.693 | 1.00 | 0.00 C |
| ATOM | 270 | О | LEU A | 23140.073 | -0.186 | 4.438 | 1.00 | 0.00 O |
| ATOM | 271 | CB | LEU A | 23141.206 | -2.070 | 6.824 | 1.00 | 0.00 C |
| ATOM . | 272 | CG | LEU A | 23141.688 | -2.224 | 8.267 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23140.698 | -3.049 | 9.075 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.069 | -2.862 | 8.302 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.463 | 0.329 | 7.434 | 1.00 | 0.00 H |
| ATOM | 276 | HA | LEU A | 23142.756 | - 0.799 | 6.074 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.126 | -2.077 | 6.823 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.555 | -2.921 | 6.259 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23141.758 | -1.248 | 8.722 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23140.860 | -4.098 | 8.880 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23139.691 | -2.781 | 8.791 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23140.840 | -2.852 | 10.127 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23143.649 | -2.423 | 9.100 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23143.568 | -2.691 | 7.359 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23142.970 | -3.924 | 8.469 | 1.00 | 0.00 H |

| ATOM | 286 | N | ALA A | 24141.859 | -1.379 | 3.768 | 1.00 | 0.00 N |
|------|-----|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 287 | CA | ALA A | 24141.447 | -1.417 | 2.370 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24141.974 | -2.668 | 1.676 | 1.00 | 0.00 C |
| ATOM | 289 | О | ALA A | 24142.870 | -3.341 | 2.186 | 1.00 | 0.00 O |
| ATOM | 290 | СВ | ALA A | 24141.925 | -0.168 | 1.646 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.693 | -1.820 | 4.032 | 1.00 | 0.00 H |
| ATOM | 292 | HA | ALAA | 24140.367 | -1.430 | 2.341 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALA A | 24141.383 | -0.061 | 0.718 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24142.981 | -0.255 | 1.439 | 1.00 | 0.00 H |
| ATOM | 295 | 3НВ | ALA A | 24141.749 | 0.698 | 2.267 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.413 | -2.975 | 0.511 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25141.827 | -4.145 | -0.252 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.061 | -3.785 | -1.716 | 1.00 | 0.00 C |
| ATOM | 299 | О | GLU A | 25141.346 | -2.961 | -2.285 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25140.773 | -5.248 | -0.147 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.270 | -6.611 | -0.600 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.237 | -7.371 | -1.407 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25139.590 | -8.277 | -0.841 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25140.072 | -7.060 | -2.605 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25140.703 | -2.399 | 0.156 | 1.00 | 0.00 H |
| ATOM | 306 | НА | GLU A | 25142.754 | -4.505 | 0.169 | 1.00 | 0.00 H |
| ATOM | 307 | 1HB | GLU A | 25140.453 | -5.328 | 0.880 | 1.00 | 0.00 H |
| ATOM | 308 | 2HB | GLU A | 25139.924 | -4.978 | -0.760 | 1.00 | 0.00 H |
| ATOM | 309 | 1HG | GLU A | 25142.151 | -6.474 | -1.210 | 1.00 | 0.00 H |
| ATOM | 310 | 2HG | GLU A | 25141.525 | -7.194 | 0.273 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.066 | -4.410 | -2.321 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.394 | -4.156 | -3.718 | 1.00 | 0.00 C |

| ATOM | 313 | C | VAL A | 26142.998 | -5.336 | -4.599 | 1.00 | 0.00 C | |
|------|-----|------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 314 | О | VALA | 26143.026 | -6.486 | -4.161 | 1.00 | 0.00 O | |
| ATOM | 315 | CB | VAL A | 26144.898 | -3.876 | -3.901 | 1.00 | 0.00 C | |
| ATOM | 316 | CG1 | VALA | 26145.188 | -3.419 | -5.322 | 1.00 | 0.00 C | |
| ATOM | 317 | CG2 | VAL A | 26145.374 | -2.841 | -2.892 | 1.00 | 0.00 C | |
| ATOM | 318 | Н | VAL A | 26143.601 | -5.057 | -1.815 | 1.00 | 0.00 H | |
| ATOM | 319 | HA | VAL A | 26142.845 | -3.282 | -4.036 | 1.00 | 0.00 H | |
| ATOM | 320 | НВ | VAL A | 26145.438 | -4.794 | -3.724 | 1.00 | 0.00 H | |
| ATOM | 321 | 1HG1 | VALA | 26144.303 | -2.967 | -5.743 | 1.00 | 0.00 H | |
| ATOM | 322 | 2HG1 | VAL A | 26145.477 | -4.270 | -5.921 | 1.00 | 0.00 H | |
| ATOM | 323 | 3HG1 | VAL A | 26145.990 | -2.697 | -5.311 | 1.00 | 0.00 H | |
| ATOM | 324 | 1HG2 | VAL A | 26145.426 | -3.291 | -1.912 | 1.00 | 0.00 H | |
| ATOM | 325 | 2HG2 | VAL A | 26144.682 | -2.013 | -2.872 | 1.00 | 0.00 H | |
| ATOM | 326 | 3HG2 | VAL A | 26146.354 | -2.485 | -3.177 | 1.00 | 0.00 H | |
| ATOM | 327 | N | LYS A | 27142.631 | -5.043 | -5.842 | 1.00 | 0.00 N | |
| ATOM | 328 | CA | LYS A | 27142.230 | -6.080 | -6.785 | 1.00 | 0.00 C | |
| ATOM | 329 | C | LYS A | 27143.429 | -6.587 | -7.579 | 1.00 | 0.00 C | |
| ATOM | 330 | О | LYS A | 27143.642 | -6.187 | -8.723 | 1.00 | 0.00 O | |
| ATOM | 331 | СВ | LYS A | 27141.161 | -5.544 | -7.739 | 1.00 | 0.00 C | |
| ATOM | 332 | CG | LYS A | 27139.740 | -5.743 | -7.235 | 1.00 | 0.00 C | |
| ATOM | 333 | CD | LYS A | 27139.084 | -6.954 | -7.879 | 1.00 | 0.00 C | |
| ATOM | 334 | CE | LYS A | 27139.179 | -8.181 | -6.985 | 1.00 | 0.00 C | |
| ATOM | 335 | NZ | LYS A | 27139.457 | -9.418 | -7.765 | 1.00 | 0.00 N | |
| ATOM | 336 | Н | LYS A | 27142.630 | -4.106 | -6.132 | 1.00 | 0.00 H | |
| ATOM | 337 | НА | LYS A | 27141.815 | -6.900 | -6.219 | 1.00 | 0.00 H | |
| ATOM | 338 | 1HB | LYS A | 27141.323 | -4.487 | -7.886 | 1.00 | 0.00 H | |
| ATOM | 339 | 2HB | LYS A | 27141.257 | -6.049 | -8.689 | 1.00 | 0.00 H | |

| ATOM | 340 1HG | LYS A | 27139.765 | -5.886 | -6.166 | 1.00 | 0.00 H |
|------|---------|-------|-------------|---------|--------|------|--------|
| ATOM | 341 2HG | LYS A | 27139.159 | -4.863 | -7.470 | 1.00 | 0.00 H |
| ATOM | 342 1HD | LYS A | 27138.044 | -6.734 | -8.061 | 1.00 | 0.00 H |
| ATOM | 343 2HD | LYS A | 27139.579 | -7.164 | -8.816 | 1.00 | 0.00 H |
| ATOM | 344 1HE | LYS A | 27139.976 | -8.030 | -6.272 | 1.00 | 0.00 H |
| ATOM | 345 2HE | LYS A | 27138.244 | -8.299 | -6.459 | 1.00 | 0.00 H |
| ATOM | 346 1HZ | LYS A | 27138.945 - | 10.223 | -7.353 | 1.00 | 0.00 H |
| ATOM | 347 2HZ | LYS A | 27140.475 | -9.627 | -7.756 | 1.00 | 0.00 H |
| ATOM | 348 3HZ | LYS A | 27139.150 | -9.294 | -8.752 | 1.00 | 0.00 H |
| ATOM | 349 N | GLU A | 28144.209 | -7.469 | -6.964 | 1.00 | 0.00 N |
| ATOM | 350 CA | GLU A | 28145.388 | -8.032 | -7.613 | 1.00 | 0.00 C |
| ATOM | 351 C | GLU A | 28145.339 | -9.556 | -7.602 | 1.00 | 0.00 C |
| ATOM | 352 O | GLU A | 28144.374 | -10.153 | -7.126 | 1.00 | 0.00 O |
| ATOM | 353 CB | GLU A | 28146.661 | -7.544 | -6.918 | 1.00 | 0.00 C |
| ATOM | 354 CG | GLU A | 28147.726 | -7.045 | -7.879 | 1.00 | 0.00 C |
| ATOM | 355 CD | GLU A | 28148.621 | -5.987 | -7.262 | 1.00 | 0.00 C |
| ATOM | 356 OE1 | GLU A | 28148.123 | -4.875 | -6.987 | 1.00 | 0.00 O |
| ATOM | 357 OE2 | GLU A | 28149.819 | -6.271 | -7.052 | 1.00 | 0.00 O |
| ATOM | 358 H | GLU A | 28143.987 | -7.749 | -6.051 | 1.00 | 0.00 H |
| ATOM | 359 HA | GLU A | 28145.396 | -7.691 | -8.638 | 1.00 | 0.00 H |
| ATOM | 360 1HB | GLU A | 28146.405 | -6.736 | -6.249 | 1.00 | 0.00 H |
| ATOM | 361 2HB | GLU A | 28147.079 | -8.356 | -6.341 | 1.00 | 0.00 H |
| ATOM | 362 1HG | GLU A | 28148.340 | -7.880 | -8.183 | 1.00 | 0.00 H |
| ATOM | 363 2HG | GLU A | 28147.241 | -6.623 | -8.748 | 1.00 | 0.00 H |
| ATOM | 364 N | ASN A | 29146.388 | -10.180 | -8.131 | 1.00 | 0.00 N |
| ATOM | 365 CA | ASN A | 29146.464 | -11.635 | -8.182 | 1.00 | 0.00 C |
| ATOM | 366 C | ASN A | 29146.473 | -12.229 | -6.774 | 1.00 | 0.00 C |

| ATOM | 367 | Ο | ASN A | 29145.597 - | 13.017 | -6.419 | 1.00 | 0.00 O |
|------|-------|------|-------|--------------|---------|---------|------|--------|
| ATOM | 368 | CB | ASN A | 29147.717 - | 12.075 | -8.943 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29147.423 - | 12.410 | -10.393 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29147.664 -1 | 3.530 - | 10.844 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29146.902 -1 | 1.437 - | 11.130 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29147.126 | -9.650 | -8.495 | 1.00 | 0.00 H |
| ATOM | 373 | НА | ASN A | 29145.590 - | 11.995 | -8.705 | 1.00 | 0.00 H |
| ATOM | 374 1 | НВ | ASN A | 29148.444 -1 | 1.278 | -8.918 | 1.00 | 0.00 H |
| ATOM | 375 2 | 2HB | ASN A | 29148.132 -1 | 2.951 | -8.467 | 1.00 | 0.00 H |
| ATOM | 376 1 | HD2 | ASN A | 29146.737 -1 | 0.570 - | 10.704 | 1.00 | 0.00 H |
| ATOM | 377 2 | 2HD2 | ASN A | 29146.701 -1 | 1.625 - | 12.071 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30147.468 - | 11.853 | -5.951 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30147.587 - | 12.350 | -4.578 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30146.604 -1 | 1.669 | -3.628 | 1.00 | 0.00 C |
| ATOM | 381 | О | PRO A | 30146.755 - | 10.489 | -3.310 | 1.00 | 0.00 O |
| ATOM | 382 | CB | PRO A | 30149.025 - | 11.990 | -4.206 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30149.325 - | 10.773 | -5.008 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30148.555 - | 10.915 | -6.295 | 1.00 | 0.00 C |
| ATOM | 385 | НА | PRO A | 30147.456 - | 13.420 | -4.531 | 1.00 | 0.00 H |
| ATOM | 386 1 | НВ | PRO A | 30149.086 -1 | 1.793 | -3.146 | 1.00 | 0.00 H |
| ATOM | 387 2 | 2HB | PRO A | 30149.682 -1 | 2.806 | -4.465 | 1.00 | 0.00 H |
| ATOM | 388 1 | HG | PRO A | 30149.001 | -9.892 | -4.474 | 1.00 | 0.00 H |
| ATOM | 389 2 | 2HG | PRO A | 30150.385 - | 10.720 | -5.212 | 1.00 | 0.00 H |
| ATOM | 390 1 | HD | PRO A | 30148.156 | -9.960 | -6.602 | 1.00 | 0.00 H |
| ATOM | 391 2 | 2HD | PRO A | 30149.186 - | 11.325 | -7.069 | 1.00 | 0.00 H |
| ATOM | 392 | N | PRO A | 31145.579 - | 12.403 | -3.156 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31144.575 - | 11.854 | -2.239 | 1.00 | 0.00 C |

| ATOM | 394 | C | PRO A | 31145.149 | -11.573 | -0.854 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 395 | O | PRO A | 31145.083 | -12.418 | 0.038 | 1.00 | 0.00 O |
| ATOM | 396 | CB | PRO A | 31143.517 | -12.957 | -2.165 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31144.253 | -14.209 | -2.491 | 1.00 | 0.00 C |
| ATOM | 398 | CD | PRO A | 31145.317 | -13.819 | -3.478 | 1.00 | 0.00 C |
| ATOM | 399 | НА | PRO A | 31144.132 | -10.951 | -2.633 | 1.00 | 0.00 H |
| ATOM | 400 | lНВ | PRO A | 31143.097 | -12.991 | -1.170 | 1.00 | 0.00 H |
| ATOM | 401 2 | 2HB | PRO A | 31142.737 | -12.761 | -2.885 | 1.00 | 0.00 H |
| ATOM | 402 | IHG | PRO A | 31144.703 | -14.614 | -1.596 | 1.00 | 0.00 H |
| ATOM | 403 2 | 2HG | PRO A | 31143.580 | -14.929 | -2.931 | 1.00 | 0.00 H |
| ATOM | 404 | HD | PRO A | 31146.205 | -14.418 | -3.334 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31144.950 | -13.923 | -4.488 | 1.00 | 0.00 H |
| ATOM | 406 | N | PHE A | 32145.712 | -10.382 | -0.683 | 1.00 | 0.00 N |
| ATOM | 407 | CA | PHE A | 32146.298 | -9.990 | 0.593 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.431 | -8.947 | 1.292 | 1.00 | 0.00 C |
| ATOM | 409 | О | PHE A | 32144.494 | -8.408 | 0.703 | 1.00 | 0.00 O |
| ATOM | 410 | СВ | PHE A | 32147.709 | -9.437 | 0.382 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32147.801 | -8.437 | -0.735 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.541 | -8.716 | -1.873 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32147.149 | -7.218 | -0.646 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.628 | -7.799 | -2.902 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.233 | -6.295 | -1.672 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32147.973 | -6.586 | -2.801 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.734 | -9.751 | -1.433 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.355 | -10.870 | 1.216 | 1.00 | 0.00 H |
| ATOM | 419 | IНВ | PHE A | 32148.038 | -8.952 | 1.289 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.377 | -10.254 | 0.155 | 1.00 | 0.00 H |

| ATOM | 421 | HD1 | PHE A | 32149.052 | -9.664 | -1.952 | 1.00 | 0.00 H |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 422 | HD2 | PHE A | 32146.571 | -6.989 | 0.237 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32149.208 | -8.027 | -3.784 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32146.719 | -5.348 | -1.590 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.039 | -5.867 | -3.604 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33145.750 | -8.668 | 2.552 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.000 | -7.690 | 3.332 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33145.940 | -6.694 | 4.004 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33146.852 | -7.081 | 4.734 | 1.00 | 0.00 O |
| ATOM | 430 | СВ | TYR A | 33144.147 | -8.395 | 4.388 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33142.780 | -8.803 | 3.888 | 1.00 | 0.00 C |
| ATOM | 432 | CDI | TYR A | 33141.996 | -7.922 | 3.154 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.273 - | 10.070 | 4.151 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33140.746 | -8.291 | 2.696 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.023 - | 10.447 | 3.696 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.264 | -9.554 | 2.970 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.019 | -9.926 | 2.514 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.508 | -9.131 | 2.967 | 1.00 | 0.00 H |
| ATOM | 439 | НА | TYR A | 33144.351 | -7.155 | 2.655 | 1.00 | 0.00 H |
| ATOM | 440 1 | НВ | TYR A | 33144.659 | -9.288 | 4.717 | 1.00 | 0.00 H |
| ATOM | 441 2 | 2HB | TYR A | 33144.010 | -7.734 | 5.230 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33142.376 | -6.934 | 2.941 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.869 - | 10.766 | 4.721 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33140.152 | -7.592 | 2.126 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.646 - | 11.436 | 3.910 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.088 | -10.756 | 2.037 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.710 | -5.410 | 3.751 | 1.00 | 0.00 N |

| ATOM | 448 | CA | GLY A | 34146.544 | -4.378 | 4.337 | 1.00 | 0.00 C |
|------|-----|------|--------|-----------|--------|-------|------|--------|
| ATOM | 449 | C | GLY A | 34145.757 | -3.138 | 4.711 | 1.00 | 0.00 C |
| ATOM | 450 | О | GLY A | 34144.578 | -3.019 | 4.378 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34144.969 | -5.161 | 3.160 | 1.00 | 0.00 H |
| ATOM | 452 | 1HA | GLY A | 34147.016 | -4.774 | 5.225 | 1.00 | 0.00 H |
| ATOM | 453 | 2HA | GLY A | 34147.312 | -4.103 | 3.628 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.409 | -2.212 | 5.406 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VAL A | 35145.764 | -0.974 | 5.827 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.453 | 0.240 | 5.212 | 1.00 | 0.00 C |
| ATOM | 457 | O | VAL A | 35147.668 | 0.241 | 5.013 | 1.00 | 0.00 O |
| ATOM | 458 | CB | VAL A | 35145.763 | -0.835 | 7.362 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.187 | -0.811 | 7.901 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VALA | 35145.001 | 0.411 | 7.788 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.348 | -2.365 | 5.642 | 1.00 | 0.00 H |
| ATOM | 462 | HA | VAL A | 35144.738 | -1.002 | 5.489 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.262 | -1.697 | 7.781 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VAL A | 35147.865 | -0.519 | 7.113 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35147.453 | -1.795 | 8.258 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VAL A | 35147.252 | -0.103 | 8.714 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | .VAL A | 35145.141 | 0.574 | 8.847 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VAL A | 35143.950 | 0.278 | 7.581 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VAL A | 35145.372 | 1.265 | 7.241 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.670 | 1.271 | 4.913 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.207 | 2.491 | 4.322 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.127 | 3.214 | 5.300 | 1.00 | 0.00 C |
| ATOM | 473 | О | ILE A | 36146.803 | 3.363 | 6.478 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.080 | 3.449 | 3.888 | 1.00 | 0.00 C |

| ATOM | 475 | CG1 | ILE A | 36144.064 | 2.715 | 3.011 | 1.00 | 0.00 C |
|------|-----|------|-------|-------------|-------|--------|------|----------|
| ATOM | 476 | CG2 | ILEA | 36145.658 | 4.648 | 3.147 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.904 | 3.583 | 2.573 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.709 | 1.210 | 5.097 | 1.00 | 0.00 H |
| ATOM | 479 | HA | ILE A | 36146.775 | 2.215 | 3.445 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.584 | 3.811 | 4.775 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.560 | 2.354 | 2.122 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.663 | 1.876 | 3.560 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36146.620 | 4.385 | 2.734 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36145.776 | 5.472 | 3.835 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36144.989 | 4.936 | 2.351 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36142.384 | 3.954 | 3.443 | 1.00 | 0.00 H |
| ATOM | 487 | 2HD1 | ILE A | 36142.225 | 2.999 | 1.970 | 1.00 | 0.00 H |
| ATOM | 488 | 3HD1 | ILE A | 36143.276 | 4.415 | 1.994 | 1.00 | 0.00 H |
| ATOM | 489 | N | ARG A | 37148.276 | 3.661 | 4.804 | 1.00 | 0.00 N |
| ATOM | 490 | CA | ARG A | A 37149.245 | 4.367 | 5.633 | 1.00 | · 0.00 C |
| ATOM | 491 | C | ARG A | 37149.477 | 5.782 | 5.116 | 1.00 | 0.00 C |
| ATOM | 492 | О | ARG A | 37149.185 | 6.761 | 5.804 | 1.00 | 0.00 O |
| ATOM | 493 | CB | ARG A | A 37150.569 | 3.602 | 5.672 | 1.00 | 0.00 C |
| ATOM | 494 | CG | ARG A | A 37150.404 | 2.115 | 5.937 | 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | A 37150.291 | 1.823 | 7.424 | 1.00 | 0.00 C |
| ATOM | 496 | NE | ARG A | 37149.079 | 2.397 | 8.006 | 1.00 | 0.00 N |
| ATOM | 497 | CZ | ARG A | 37148.908 | 2.602 | 9.309 | 1.00 | 0.00 C |
| ATOM | 498 | NHI | ARG A | 37149.866 | 2.280 | 10.170 | 1.00 | 0.00 N |
| ATOM | 499 | NH2 | ARG A | 37147.775 | 3.129 | 9.754 | 1.00 | 0.00 N |
| ATOM | 500 | Н | ARG A | 37148.478 | 3.510 | 3.857 | 1.00 | 0.00 H |
| ATOM | 501 | НА | ARG A | A 37148.844 | 4.424 | 6.635 | 1.00 | 0.00 H |

| ATOM | 502 | 1HB | ARG A | 37151.068 | 3.724 | 4.723 | 1.00 | 0.00 H |
|------|-------|-------|-------|-----------|--------|--------|------|--------|
| ATOM | 503 2 | 2HB | ARG A | 37151.188 | 4.018 | 6.452 | 1.00 | 0.00 H |
| ATOM | 504 | 1HG | ARG A | 37149.508 | 1.768 | 5.443 | 1.00 | 0.00 H |
| ATOM | 505 2 | 2HG | ARG A | 37151.261 | 1.592 | 5.540 | 1.00 | 0.00 H |
| ATOM | 506 | 1HD | ARG A | 37150.274 | 0.753 | 7.568 | 1.00 | 0.00 H |
| ATOM | 507 2 | 2HD | ARG A | 37151.152 | 2.240 | 7.926 | 1.00 | 0.00 H |
| ATOM | 508 | HE | ARG A | 37148.356 | 2.643 | 7.392 | 1.00 | 0.00 H |
| ATOM | 509 | 1HH1. | ARG A | 37150.722 | 1.882 | 9.843 | 1.00 | 0.00 H |
| ATOM | 510 2 | 2HH1. | ARG A | 37149.730 | 2.437 | 11.149 | 1.00 | 0.00 H |
| ATOM | 511 | 1HH2. | ARG A | 37147.050 | 3.372 | 9.109 | 1.00 | 0.00 H |
| ATOM | 512 2 | 2HH2 | ARG A | 37147.646 | 3.282 | 10.734 | 1.00 | 0.00 H |
| ATOM | 513 | N | TRPA | 38150.004 | 5.886 | 3.900 | 1.00 | 0.00 N |
| ATOM | 514 | CA | TRPA | 38150.274 | 7.185 | 3.294 | 1.00 | 0.00 C |
| ATOM | 515 | C | TRPA | 38149.557 | 7.323 | 1.954 | 1.00 | 0.00 C |
| ATOM | 516 | О | TRPA | 38149.618 | 6.430 | 1.110 | 1.00 | 0.00 O |
| ATOM | 517 | CB | TRPA | 38151.783 | 7.382 | 3.104 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38152.128 | 8.579 | 2.267 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRPA | 38152.387 | 9.844 | 2.710 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRPA | 38152.247 | 8.620 | 0.840 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRPA | 38152.659 | 10.670 | 1.646 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.579 | 9.941 | 0.486 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38152.104 | 7.668 | -0.174 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRPA | 38152.771 | 10.333 | -0.836 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.296 | 8.057 | -1.486 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRP A | 38152.625 | 9.380 | -1.807 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRP A | 38150.216 | 5.071 | 3.400 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRPA | 38149.904 | 7.945 | 3.964 | 1.00 | 0.00 H |

| ATOM | 529 1 | lНВ | TRPA | 38152.247 | 7.508 | 4.071 | 1.00 | 0.00 H |
|------|--------------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 530 2 | 2HB | TRP A | 38152.195 | 6.507 | 2.623 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRP A | 38152.376 | 10.139 | 3.748 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRP A | 38152.875 | 11.623 | 1.706 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRP A | 38151.850 | 6.644 | 0.055 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRP A | 38153.022 | 11.349 | -1.102 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.189 | 7.335 | -2.281 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRP A | 38152.765 | 9.638 | -2.847 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.889 | 8.456 | 1.765 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39148.169 | 8.727 | 0.528 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILE A | 39148.631 | 10.044 | -0.083 | 1.00 | 0.00 C |
| ATOM | 540 | O | ILE A | 39148.297 | 11.119 | 0.414 | 1.00 | 0.00 O |
| ATOM | 541 | СВ | ILE A | 39146.647 | 8.785 | 0.762 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39146.181 | 7.562 | 1.554 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.911 | 8.876 | -0.567 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.818 | 7.736 | 2.187 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.887 | 9.132 | 2.475 | 1.00 | 0.00 H |
| ATOM | 546 | HA | ILE A | 39148.378 | 7.924 | -0.165 | 1.00 | 0.00 H |
| ATOM | 547 | HB | ILE A | 39146.427 | 9.678 | 1.328 | 1.00 | 0.00 H |
| ATOM | 548 | IHG1 | ILE A | 39146.134 | 6.710 | 0.893 | 1.00 | 0.00 H |
| ATOM | 549 2 | HG1 | ILE A | 39146.891 | 7.360 | 2.342 | 1.00 | 0.00 H |
| ATOM | 550 | lHG2 | ILE A | 39146.058 | 9.857 | -0.994 | 1.00 | 0.00 H |
| ATOM | 551 2 | 2HG2 | ILE A | 39144.856 | 8.708 | -0.405 | 1.00 | 0.00 H |
| ATOM | 552 3 | 3HG2 | ILE A | 39146.295 | 8.127 | -1.243 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.725 | 8.742 | 2.569 | 1.00 | 0.00 H |
| ATOM | 554 2 | 2HD1 | ILE A | 39144.706 | 7.032 | 2.998 | 1.00 | 0.00 H |
| ATOM | 555 3 | 3HD1 | ILE A | 39144.052 | 7.559 | 1.446 | 1.00 | 0.00 H |

| ATOM | 556 | N | GLY A | 40149.407 | 9.955 | -1.159 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 557 | CA | GLY A | 40149.906 | 11.152 | -1.808 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.448 | 10.884 | -3.197 | 1.00 | 0.00 C |
| ATOM | 559 | O | GLY A | 40150.274 | 9.794 | -3.742 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.646 | 9.072 | -1.510 | 1.00 | 0.00 H |
| ATOM | 561 1 | ΙHΑ | GLY A | 40149.104 | 11.870 | -1.880 | 1.00 | 0.00 H |
| ATOM | 562 2 | 2HA | GLY A | 40150.693 | 11.572 | -1.202 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41151.109 | 11.884 | -3.769 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.683 | 11.763 | -5.103 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41153.162 | 12.148 | -5.090 | 1.00 | 0.00 C |
| ATOM | 566 | O | GLN A | 41153.506 | 13.302 | -4.830 | 1.00 | 0.00 O |
| ATOM | 567 | СВ | GLN A | 41150.919 | 12.654 | -6.082 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41149.411 | 12.488 | -6.004 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.672 | 13.804 | -6.138 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.635 | 14.607 | -5.206 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41148.077 | 14.033 | -7.304 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41151.213 | 12.728 | -3.282 | 1.00 | 0.00 H |
| ATOM | 573 | HA | GLN A | 41151.588 | 10.735 | -5.415 | 1.00 | 0.00 H |
| ATOM | 574 1 | IHB | GLN A | 41151.157 | 13.685 | -5.871 | 1.00 | 0.00 H |
| ATOM | 575 2 | 2HB | GLN A | 41151.235 | 12.418 | -7.086 | 1.00 | 0.00 H |
| ATOM | 576 1 | lHG | GLN A | 41149.090 | 11.832 | -6.799 | 1.00 | 0.00 H |
| ATOM | 577 2 | 2HG | GLN A | 41149.158 | 12.046 | -5.051 | 1.00 | 0.00 H |
| ATOM | 578 | HE2 | GLN A | 41148.148 | 13.349 | -8.000 | 1.00 | 0.00 H |
| ATOM | 579 2 | 2HE2 | GLN A | 41147.594 | 14.878 | -7.418 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42154.062 | 11.187 | -5.368 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.507 | 11.441 | -5.381 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.892 | 12.546 | -6.360 | 1.00 | 0.00 C |

| ATOM | 583 O | PRO A | 42155.139 | 12.859 | -7.283 | 1.00 | 0.00 O |
|------|---------|-------|-----------|--------|---------|------|--------|
| ATOM | 584 CB | PRO A | 42156.107 | 10.102 | -5.822 | 1.00 | 0.00 C |
| ATOM | 585 CG | PRO A | 42155.065 | 9.090 | -5.491 | 1.00 | 0.00 C |
| ATOM | 586 CD | PRO A | 42153.749 | 9.784 | -5.689 | 1.00 | 0.00 C |
| ATOM | 587 HA | PRO A | 42155.871 | 11.695 | -4.396 | 1.00 | 0.00 H |
| ATOM | 588 1HB | PRO A | 42156.311 | 10.129 | -6.882 | 1.00 | 0.00 H |
| ATOM | 589 2HB | PRO A | 42157.022 | 9.918 | -5.279 | 1.00 | 0.00 H |
| ATOM | 590 1HG | PRO A | 42155.148 | 8.245 | -6.157 | 1.00 | 0.00 H |
| ATOM | 591 2HG | PRO A | 42155.173 | 8.774 | -4.464 | 1.00 | 0.00 H |
| ATOM | 592 1HD | PRO A | 42153.419 | 9.686 | -6.713 | 1.00 | 0.00 H |
| ATOM | 593 2HD | PRO A | 42153.007 | 9.389 | -5.010 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43157.076 | 13.153 | -6.172 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.559 | 14.227 | -7.043 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43157.974 | 13.715 | -8.417 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43159.140 | 13.389 | -8.642 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43158.771 | 14.776 | -6.291 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43159.256 | 13.633 | -5.468 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43158.034 | 12.839 | -5.096 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43156.820 | 15.006 | -7.159 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43159.519 | 15.100 | -7.000 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43158.469 | 15.608 | -5.673 | 1.00 | 0.00 H |
| ATOM | 604 1HG | PRO A | 43159.935 | 13.027 | -6.048 | 1.00 | 0.00 H |
| ATOM | 605 2HG | PRO A | 43159.747 | 14.004 | -4.580 | 1.00 | 0.00 H |
| ATOM | 606 1HD | PRO A | 43158.262 | 11.783 | -5.079 | 1.00 | 0.00 H |
| ATOM | 607 2HD | PRO A | 43157.654 | 13.158 | -4.137 | 1.00 | 0.00 H |
| ATOM | 608 N | GLY A | 44157.015 | 13.646 | -9.332 | 1.00 | 0.00 N |
| ATOM | 609 CA | GLY A | 44157.304 | 13.172 | -10.672 | 1.00 | 0.00 C |

| ATOM | 610 | C | GLY A | 44156.071 | 12.647 -11.380 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|----------------|------|--------|
| ATOM | 611 | O | GLY A | 44155.783 | 13.041 -12.510 | 1.00 | 0.00 O |
| ATOM | 612 | Н | GLY A | 44156.104 | 13.919 -9.097 | 1.00 | 0.00 H |
| ATOM | 613 | 1HA | GLY A | 44157.716 | 13.985 -11.248 | 1.00 | 0.00 H |
| ATOM | 614 | 2HA | GLY A | 44158.035 | 12.380 -10.612 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45155.344 | 11.756 -10.716 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEU A | 45154.136 | 11.177 -11.291 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45152.926 | 11.462 -10.410 | 1.00 | 0.00 C |
| ATOM | 618 | O | LEU A | 45152.826 | 10.948 -9.296 | 1.00 | 0.00 O |
| ATOM | 619 | СВ | LEU A | 45154.307 | 9.668 -11.472 | 1.00 | 0.00 C |
| ATOM | 620 | CG | LEU A | 45154.840 | 8.927 -10.245 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.467 | 7.451 -10.307 | 1.00 | 0.00 C |
| ATOM | 622 | CD2 | LEU A | 45156.350 | 9.096 -10.132 | 1.00 | 0.00 C |
| ATOM | 623 | Н | LEU A | 45155.624 | 11.483 -9.816 | 1.00 | 0.00 H |
| ATOM | 624 | НА | LEU A | 45153.977 | 11.632 -12.258 | 1.00 | 0.00 H |
| ATOM | 625 | 1HB | LEU A | 45153.346 | 9.248 -11.733 | 1.00 | 0.00 H |
| ATOM | 626 | 2HB | LEU A | 45154.989 | 9.500 -12.292 | 1.00 | 0.00 H |
| ATOM | 627 | HG | LEU A | 45154.389 | 9.345 -9.357 | 1.00 | 0.00 H |
| ATOM | 628 | 1HD1 | LEU A | 45153.870 | 7.266 -11.188 | 1.00 | 0.00 H |
| ATOM | 629 | 2HD1 | LEU A | 45153.901 | 7.186 -9.427 | 1.00 | 0.00 H |
| ATOM | 630 | 3HD1 | LEU A | 45155.365 | 6.852 -10.350 | 1.00 | 0.00 H |
| ATOM | 631 | 1HD2 | LEU A | 45156.683 | 9.843 -10.837 | 1.00 | 0.00 H |
| ATOM | 632 | 2HD2 | LEU A | 45156.836 | 8.157 -10.349 | 1.00 | 0.00 H |
| ATOM | 633 | 3HD2 | LEU A | 45156.602 | 9.408 -9.130 | 1.00 | 0.00 H |
| ATOM | 634 | N | ASN A | 46152.008 | 12.282 -10.911 | 1.00 | 0.00 N |
| ATOM | 635 | CA | ASN A | 46150.810 | 12.622 -10.156 | 1.00 | 0.00 C |
| ATOM | 636 | C | ASN A | 46149.846 | 11.443 -10.124 | 1.00 | 0.00 C |

| ATOM | 637 | O | ASN A | 46149.218 | 11.110 - | 11.130 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|----------|----------------|------|--------|
| ATOM | 638 | СВ | ASN A | 46150.123 | 13.843 - | -10.773 | 1.00 | 0.00 C |
| ATOM | 639 | CG | ASN A | 46149.380 | 14.670 | -9.743 | 1.00 | 0.00 C |
| ATOM | 640 | OD1 | ASN A | 46149.955 | 15.100 | -8.743 | 1.00 | 0.00 O |
| ATOM | 641 | ND2 | ASN A | 46148.095 | 14.900 | -9.984 | 1.00 | 0.00 N |
| ATOM | 642 | Н | ASN A | 46152.139 | 12.664 - | 11.804 | 1.00 | 0.00 H |
| ATOM | 643 | HA | ASN A | 46151.108 | 12.858 | -9.146 | 1.00 | 0.00 H |
| ATOM | 644 | 1HB | ASN A | 46150.868 | 14.469 - | 11.241 | 1.00 | 0.00 H |
| ATOM | 645 | 2HB | ASN A | 46149.417 | 13.511 - | 11.519 | 1.00 | 0.00 H |
| ATOM | 646 | 1HD2 | ASN A | 46147.703 | 14.526 - | 10.801 | 1.00 | 0.00 H |
| ATOM | 647 | 2HD2 | ASN A | 46147.590 | 15.433 | -9.335 | 1.00 | 0.00 H |
| ATOM | 648 | N | GLU A | 47149.734 | 10.813 | -8.961 | 1.00 | 0.00 N |
| ATOM | 649 | CA | GLU A | 47148.848 | 9.668 | -8.790 | 1.00 | 0.00 C |
| ATOM | 650 | C | GLU A | 47148.661 | 9.345 | -7.312 | 1.00 | 0.00 C |
| ATOM | 651 | O | GLU A | 47149.627 | 9.062 | -6.604 | 1.00 | 0.00 O |
| ATOM | 652 | CB | GLU A | 47149.405 | 8.446 | -9.525 | 1.00 | 0.00 C |
| ATOM | 653 | CG | GLU A | 47150.918 | 8.314 | -9.439 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.479 | 7.357 | -10.472 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.460 | 7.702 - | 11.672 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.937 | 6.263 - | 10.082 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47150.262 | 11.125 | -8.197 | 1.00 | 0.00 H |
| ATOM | 658 | HA | GLU A | 47147.889 | 9.926 | -9.214 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.964 | 7.555 | - 9.103 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47149.131 | 8.513 - | 10.568 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47151.360 | 9.285 | -9.592 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47151.180 | 7.952 | -8.455 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.416 | 9.382 | -6.851 | 1.00 | 0.00 N |

| ATOM | 664 | CA | VALA | 48147.116 | 9.085 | -5.457 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 665 | C | VAL A | 48147.475 | 7.642 | -5.124 | 1.00 | 0.00 C |
| ATOM | 666 | O | VAL A | 48146.726 | 6.717 | -5.438 | 1.00 | 0.00 O |
| ATOM | 667 | CB | VAL A | 48145.629 | 9.320 | -5.137 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VALA | 48145.378 | 9.198 | -3.642 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VAL A | 48145.180 | 10.679 | -5.652 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.684 | 9.609 | -7.462 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.709 | 9.745 | -4.840 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48145.048 | 8.560 | -5.639 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VALA | 48144.420 | 9.634 | -3.401 | 1.00 | 0.00 H |
| ATOM | 674 2 | 2HG1 | VALA | 48146.156 | 9.719 | -3.103 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VALA | 48145.381 | 8.155 | -3.360 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VALA | 48144.227 | 10.934 | -5.213 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48145.083 | 10.644 | -6.726 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VALA | 48145.912 | 11.426 | -5.381 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.629 | 7.455 | -4.492 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49149.088 | 6.123 | -4.122 | 1.00 | 0.00 C |
| ATOM | 681 | C | LEU A | 49148.955 | 5.904 | -2.621 | 1.00 | 0.00 C |
| ATOM | 682 | О | LEU A | 49149.633 | 6.554 | -1.825 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.544 | 5.923 | -4.550 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.801 | 6.069 | -6.051 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49152.275 | 6.335 | -6.317 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEU A | 49150.342 | 4.822 | -6.793 | 1.00 | 0.00 C |
| ATOM | 687 | Н | LEU A | 49149.185 | 8.231 | -4.270 | 1.00 | 0.00 H |
| ATOM | 688 | НА | LEU A | 49148.470 | 5.404 | -4.636 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49151.153 | 6.649 | -4.030 | 1.00 | 0.00 H |
| ATOM | 690 2 | 2HB | LEU A | 49150.854 | 4.935 | -4.249 | 1.00 | 0.00 H |

| ATOM | 691 | HG | LEU A | 49150.237 | 6.910 | -6.427 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 692 | 1HD1 | LEU A | 49152.707 | 6.843 | -5.468 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49152.376 | 6.954 | -7.197 | 1.00 | 0.00 H |
| ATOM | 694 | 3HD1 | LEU A | 49152.788 | 5.398 | -6.475 | 1.00 | 0.00 H |
| ATOM | 695 | 1HD2 | LEU A | 49151.185 | 4.165 | -6.951 | 1.00 | 0.00 H |
| ATOM | 696 | 2HD2 | LEU A | 49149.921 | 5.104 | -7.746 | 1.00 | 0.00 H |
| ATOM | 697 | 3HD2 | LEU A | 49149.593 | 4.311 | -6.206 | 1.00 | 0.00 H |
| ATOM | 698 | N | ALA A | 50148.077 | 4.984 | -2.240 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.856 | 4.682 | -0.832 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALA A | 50148.756 | 3.542 | -0.369 | 1.00 | 0.00 C |
| ATOM | 701 | O | ALA A | 50148.624 | 2.408 | -0.830 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.395 | 4.337 | -0.589 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.565 | 4.497 | -2.920 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50148.093 | 5.570 | -0.265 | 1.00 | 0.00 H |
| ATOM | 705 | 1HB | ALA A | 50145.792 | 4.740 | -1.389 | 1.00 | 0.00 H |
| ATOM | 706 | 2HB | ALA A | 50146.077 | 4.763 | 0.352 | 1.00 | 0.00 H |
| ATOM | 707 | 3HB | ALA A | 50146.278 | 3.265 | -0.556 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.671 | 3.850 | 0.545 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.578 | 2.839 | 1.056 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51149.878 | 1.821 | 1.933 | 1.00 | 0.00 C |
| ATOM | 711 | O | GLY A | 51149.350 | 2.162 | 2.991 | 1.00 | 0.00 O |
| ATOM | 712 | H | GLY A | 51149.730 | 4.770 | 0.876 | 1.00 | 0.00 H |
| ATOM | 713 | 1HA | GLY A | 51151.034 | 2.326 | 0.221 | 1.00 | 0.00 H |
| ATOM | 714 | 2HA | GLY A | 51151.352 | 3.324 | 1.631 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.873 | 0.567 | 1.494 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.232 | -0.504 | 2.247 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.270 | -1.379 | 2.943 | 1.00 | 0.00 C |

| | | | | - 233 | - | | | |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 718 | O | LEU A | 52151.305 | -1.710 | 2.364 | 1.00 | 0.00 O |
| ATOM | 719 | СВ | LEU A | 52148.365 | -1.360 | 1.322 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.140 | -0.650 | 0.742 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.534 | -1.469 | -0.388 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52146.108 | -0.394 | 1.830 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.311 | 0.356 | 0.643 | 1.00 | 0.00 H |
| ATOM | 724 | НА | LEU A | 52148.601 | -0.050 | 2.997 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.980 | -1.701 | 0.501 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52148.024 | -2.221 | 1.876 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.444 | 0.305 | 0.336 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52145.929 | -0.828 | -1.012 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52145.918 | -2.253 | 0.027 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52147.324 | -1.906 | -0.979 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52146.587 | 0.078 | 2.675 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52145.673 | -1.332 | 2.141 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52145.334 | 0.254 | 1.447 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53149.985 | -1.750 | 4.187 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.892 | -2.587 | 4.962 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.367 | -4.015 | 5.058 | 1.00 | 0.00 C |
| ATOM | 737 | Ο | GLU A | 53149.392 | -4.282 | 5.759 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.084 | -2.006 | 6.365 | 1.00 | 0.00 C |
| ATOM | 739 | CG | GLU A | 53152.053 | -2.799 | 7.225 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.694 | -2.758 | 8.697 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53152.597 | -2.965 | 9.535 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53150.510 | -2.518 | 9.013 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53149.143 | -1.454 | 4.594 | 1.00 | 0.00 H |
| ATOM | 744 | HA | GLU A | 53151.846 | -2.599 | 4.455 | 1.00 | 0.00 H |

| ATOM | 745 1HE | GLU A | 53151.457 | -0.996 | 6.276 | 1.00 | 0.00 H |
|------|---------|----------|-----------|--------|-------|------|--------|
| ATOM | 746 2HE | GLU A | 53150.127 | -1.982 | 6.865 | 1.00 | 0.00 H |
| ATOM | 747 1HC | G GLU A | 53152.046 | -3.828 | 6.898 | 1.00 | 0.00 H |
| ATOM | 748 2HC | G GLU A | 53153.045 | -2.389 | 7.100 | 1.00 | 0.00 H |
| ATOM | 749 N | LEU A | 54151.021 | -4.929 | 4.348 | 1.00 | 0.00 N |
| ATOM | 750 CA | A LEUA | 54150.618 | -6.331 | 4.353 | 1.00 | 0.00 C |
| ATOM | 751 C | LEU A | 54150.983 | -6.997 | 5.676 | 1.00 | 0.00 C |
| ATOM | 752 O | LEU A | 54152.069 | -6.783 | 6.212 | 1.00 | 0.00 O |
| ATOM | 753 CI | B LEUA | 54151.282 | -7.078 | 3.194 | 1.00 | 0.00 C |
| ATOM | 754 CC | G LEUA | 54151.184 | -6.382 | 1.835 | 1.00 | 0.00 C |
| ATOM | 755 CI | D1 LEU A | 54152.187 | -6.976 | 0.859 | 1.00 | 0.00 C |
| ATOM | 756 CI | D2 LEU A | 54149.771 | -6.491 | 1.283 | 1.00 | 0.00 C |
| ATOM | 757 H | LEU A | 54151.791 | -4.655 | 3.808 | 1.00 | 0.00 H |
| ATOM | 758 H | A LEUA | 54149.547 | -6.369 | 4.227 | 1.00 | 0.00 H |
| ATOM | 759 1HE | B LEUA | 54152.327 | -7.213 | 3.433 | 1.00 | 0.00 H |
| ATOM | 760 2HE | B LEUA | 54150.821 | -8.050 | 3.109 | 1.00 | 0.00 H |
| ATOM | 761 H | G LEUA | 54151.417 | -5.334 | 1.957 | 1.00 | 0.00 H |
| ATOM | 762 1HD | DI LEU A | 54151.706 | -7.745 | 0.272 | 1.00 | 0.00 H |
| ATOM | 763 2HE | D1 LEU A | 54153.012 | -7.406 | 1.407 | 1.00 | 0.00 H |
| ATOM | 764 3HE | DI LEU A | 54152.555 | -6.200 | 0.205 | 1.00 | 0.00 H |
| ATOM | 765 1HE | D2 LEU A | 54149.795 | -6.380 | 0.209 | 1.00 | 0.00 H |
| ATOM | 766 2HI | 2 LEU A | 54149.156 | -5.713 | 1.712 | 1.00 | 0.00 H |
| ATOM | 767 3HI | 2 LEU A | 54149.359 | -7.457 | 1.536 | 1.00 | 0.00 H |
| ATOM | 768 N | GLU A | 55150.065 | -7.806 | 6.197 | 1.00 | 0.00 N |
| ATOM | 769 CA | A GLUA | 55150.290 | -8.504 | 7.458 | 1.00 | 0.00 C |
| ATOM | 770 C | GLU A | 55151.347 | -9.593 | 7.295 | 1.00 | 0.00 C |
| ATOM | 771 O | GLU A | 55152.090 | -9.894 | 8.229 | 1.00 | 0.00 O |

| ATOM | 772 | CB | GLU A | 55148.983 | -9.117 | 7.965 | 1.00 | 0.00 C |
|------|--------------|-----|-------|-------------|----------------|-------|------|--------|
| ATOM | 773 | CG | GLU A | 55147.843 | -8.118 | 8.067 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55147.017 | -8.302 | 9.326 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55147.071 | -9.401 | 9.916 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55146.318 | -7.346 | 9.722 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.218 | -7.937 | 5.723 | 1.00 | 0.00 H |
| ATOM | 778 | НА | GLU A | 55150.642 | -7.782 | 8.179 | 1.00 | 0.00 H |
| ATOM | 779 1 | НВ | GLU A | 55148.683 | - 9.906 | 7.291 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55149.154 | -9.538 | 8.945 | 1.00 | 0.00 H |
| ATOM | 781 | HG | GLU A | 55148.254 | -7.120 | 8.069 | 1.00 | 0.00 H |
| ATOM | 782 2 | 2HG | GLU A | 55147.198 | -8.239 | 7.210 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56151.406 - | 10.179 | 6.103 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASPA | 56152.372 - | 11.234 | 5.818 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASPA | 56153.664 - | 10.651 | 5.256 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASPA | 56153.650 | -9.931 | 4.258 | 1.00 | 0.00 O |
| ATOM | 787 | СВ | ASPA | 56151.781 - | 12.241 | 4.830 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56150.691 | -13.091 | 5.453 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASPA | 56149.769 - | 13.504 | 4.718 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56150.759 - | 13.342 | 6.674 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.786 | -9.895 | 5.399 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.593 | -11.741 | 6.745 | 1.00 | 0.00 H |
| ATOM | 793 1 | IHB | ASPA | 56151.362 - | 11.708 | 3.990 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASPA | 56152.566 - | 12.895 | 4.480 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.781 | -10.966 | 5.905 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57156.083 | -10.474 | 5.470 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.427 | -10.999 | 4.080 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57156.851 | -12.145 | 3.927 | 1.00 | 0.00 O |

| ATOM | 799 | CB | GLU A | 57157.167 | -10.886 | 6.467 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|--------|------|---------|
| ATOM | 800 | CG | GLU A | 57157.113 | -10.116 | 7.776 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57157.985 | -10.733 | 8.852 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57158.567 | -9.973 | 9.653 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57158.086 - | 11.977 | 8.892 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.728 | -11.545 | 6.694 | 1.00 | 0.00 H |
| ATOM | 805 | НА | GLU A | 57156.033 | -9.396 | 5.431 | 1.00 | 0.00 H |
| ATOM | 806 1 | НВ | GLU A | 57157.056 - | 11.937 | 6.687 | 1.00 | 0.00 H |
| ATOM | 807 2 | ΣНВ | GLU A | 57158.135 - | 10.721 | 6.017 | 1.00 | 0.00 H |
| ATOM | 808 1 | lHG | GLU A | 57157.448 | -9.105 | 7.599 | 1.00 | 0.00 H |
| ATOM | 809 2 | 2HG | GLU A | 57156.092 - | 10.099 | 8.127 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58156.242 - | 10.156 | 3.070 | 1.00 | 0.00 N |
| ATOM | 811 | CA | CYSA | 58156.533 - | 10.535 | 1.693 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58157.946 - | 10.114 | 1.300 | 1.00 | 0.00 C |
| ATOM | 813 | О | CYS A | 58158.303 | -8.939 | 1.397 | 1.00 | 0.00 O |
| ATOM | 814 | СВ | CYS A | 58155.516 | -9.904 | 0.742 | 1.00 | ,0.00 C |
| ATOM | 815 | SG | CYS A | 58154.053 - | 10.924 | 0.443 | 1.00 | 0.00 S |
| ATOM | 816 | Н | CYS A | 58155.901 | -9.256 | 3.256 | 1.00 | 0.00 H |
| ATOM | 817 | HA | CYSA | 58156.460 | -11.611 | 1.623 | 1.00 | 0.00 H |
| ATOM | 818 1 | HB | CYS A | 58155.181 | -8.965 | 1.156 | 1.00 | 0.00 H |
| ATOM | 819 2 | 2HB | CYS A | 58155.991 | -9.722 | -0.212 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYS A | 58153.934 | -10.999 | -0.506 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALA A | 59158.744 | -11.079 | 0.855 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALA A | 59160.117 | -10.807 | 0.448 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59160.156 | -9.970 | -0.826 | 1.00 | 0.00 C |
| ATOM | 824 | O | ALA A | 59159.813 | -10.450 | -1.907 | 1.00 | 0.00 O |
| ATOM | 825 | СВ | ALAA | 59160.876 | -12.111 | 0.249 | 1.00 | 0.00 C |

| ATOM | 826 | Н | ALA A | 59158.402 - | 11.995 | 0.801 | 1.00 | 0.00 H |
|------|-------|------------|-------|-------------|---------|--------|------|--------|
| ATOM | 827 | НА | ALA A | 59160.598 | -10.256 | 1.243 | 1.00 | 0.00 H |
| ATOM | 828 | lНВ | ALA A | 59160.889 - | 12.363 | -0.801 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59160.387 - | 12.900 | 0.802 | 1.00 | 0.00 H |
| ATOM | 830 3 | ВНВ | ALA A | 59161.889 - | 11.995 | 0.605 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60160.576 | -8.716 | -0.692 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60160.651 | -7.832 | -1.840 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60160.053 | -6.468 | -1.563 | 1.00 | 0.00 C |
| ATOM | 834 | О | GLY A | 60160.466 | -5.470 | -2.152 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60160.836 | -8.388 | 0.194 | 1.00 | 0.00 H |
| ATOM | 836 | ΙHΑ | GLY A | 60161.688 | -7.708 | -2.117 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60160.122 | -8.286 | -2.665 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61159.074 | -6.425 | -0.664 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.416 | -5.173 | -0.311 | 1.00 | 0.00 C |
| ATOM | 840 | C . | CYS A | 61159.344 | -4.284 | 0.510 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.455 | -4.683 | 0.860 | 1.00 | 0.00 O |
| ATOM | 842 | СВ | CYS A | 61157.132 | -5.451 | 0.472 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYS A | 61156.021 | -6.631 | -0.329 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.788 | -7.255 | -0.229 | 1.00 | 0.00 H |
| ATOM | 845 | НА | CYS A | 61158.164 | -4.661 | -1.227 | 1.00 | 0.00 H |
| ATOM | 846 | lНВ | CYS A | 61157.389 | -5.850 | 1.442 | 1.00 | 0.00 H |
| ATOM | 847 2 | 2HB | CYS A | 61156.591 | -4.525 | 0.602 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61155.639 | -7.189 | 0.354 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.881 | -3.076 | 0.816 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.669 | -2.129 | 1.596 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.163 | -2.056 | 3.034 | 1.00 | 0.00 C |
| ATOM | 852 | O | THR A | 62158.177 | -2.701 | 3.389 | 1.00 | 0.00 O |

| ATOM | 853 | CB | THR A | 62159.619 | -0.742 | 0.955 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 854 | OG1 | THR A | 62158.314 | -0.454 | 0.483 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.573 | -0.585 | -0.208 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62157.987 | -2.815 | 0.509 | 1.00 | 0.00 H |
| ATOM | 857 | НА | THR A | 62160.691 | -2.476 | 1.603 | 1.00 | 0.00 H |
| ATOM | 858 | HB | THR A | 62159.881 | -0.003 | 1.699 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62157.782 | -0.107 | 1.204 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62160.889 | -1.560 | -0.549 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62161.435 | -0.018 | 0.108 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62160.076 | -0.066 | -1.014 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63159.847 | -1.268 | 3.857 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASPA | 63159.467 | -1.109 | 5.255 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.836 | 0.257 | 5.497 | 1.00 | 0.00 C |
| ATOM | 866 | O | ASPA | 63158.965 | 0.829 | 6.578 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASPA | 63160.689 | -1.287 | 6.160 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.787 | -0.290 | 5.849 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63162.647 | -0.600 | 4.998 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63161.789 | 0.801 | 6.458 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASPA | 63160.625 | -0.779 | 3.514 | 1.00 | 0.00 H |
| ATOM | 872 | НА | ASPA | 63158.743 | -1.875 | 5.490 | 1.00 | 0.00 H |
| ATOM | 873 | 1HB | ASPA | 63160.388 | -1.156 | 7.188 | 1.00 | 0.00 H |
| ATOM | 874 | 2HB | ASPA | 63161.083 | -2.284 | 6.029 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64158.152 | 0.775 | 4.482 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.511 | 2.071 | 4.603 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64158.215 | 3.146 | 3.799 | 1.00 | 0.00 C |
| ATOM | 878 | Ο | GLY A | 64158.375 | 4.274 | 4.263 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64158.083 | 0.274 | 3.642 | 1.00 | 0.00 H |

| ATOM | 880 | l HA | GLY A | 64156.490 | 1.989 | 4.257 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|-------|--------|------|--------|
| ATOM | 881 2 | 2HA | GLY A | 64157.505 | 2.362 | 5.643 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.638 | 2.795 | 2.589 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.329 | 3.737 | 1.717 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65158.943 | 3.515 | 0.260 | 1.00 | 0.00 C |
| ATOM | 885 | О | THR A | 65159.044 | 2.402 | -0.257 | 1.00 | 0.00 O |
| ATOM | 886 | СВ | THR A | 65160.844 | 3.600 | 1.884 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.250 | 2.258 | 1.686 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.338 | 4.034 | 3.246 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.481 | 1.880 | 2.275 | 1.00 | 0.00 H |
| ATOM | 890 | НА | THR A | 65159.034 | 4.734 | 2.008 | 1.00 | 0.00 H |
| ATOM | 891 | HB | THR A | 65161.334 | 4.215 | 1.143 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65160.827 | 1.907 | 0.900 | 1.00 | 0.00 H |
| ATOM | 893 | HG2 | THR A | 65160.554 | 4.569 | 3.761 | 1.00 | 0.00 H |
| ATOM | 894 2 | 2HG2 | THR A | 65162.197 | 4.679 | 3.129 | 1.00 | 0.00 H |
| ATOM | 895 3 | 3HG2 | THR A | 65161.619 | 3.164 | 3.822 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.503 | 4.581 | -0.399 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.101 | 4.504 | -1.799 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.101 | 5.230 | -2.694 | 1.00 | 0.00 C |
| ATOM | 899 | O | PHE A | 66159.198 | 6.457 | -2.665 | 1.00 | 0.00 O |
| ATOM | 900 | CB | PHE A | 66156.705 | 5.101 | -1.985 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.083 | 4.770 | -3.311 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.689 | 5.778 | -4.177 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.893 | 3.452 | -3.692 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.116 | 5.476 | -5.398 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.321 | 3.144 | -4.912 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.932 | 4.158 | -5.766 | 1.00 | 0.00 C |

| ATOM | 907 | Н | PHE A | 66158.446 | 5.442 | 0.066 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|-------|---------|------|--------|
| ATOM | 908 | HA | PHE A | 66158.077 | 3.461 | -2.080 | 1.00 | 0.00 H |
| ATOM | 909 | 1HB | PHE A | 66156.055 | 4.726 | -1.211 | 1.00 | 0.00 H |
| ATOM | 910 2 | 2HB | PHE A | 66156.768 | 6.176 | -1.906 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66155.833 | 6.809 | -3.891 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.196 | 2.659 | - 3.026 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66154.813 | 6.271 | -6.064 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.178 | 2.112 | -5.197 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.485 | 3.919 | -6.720 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.843 | 4.465 | -3.487 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67160.835 | 5.035 | -4.390 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.898 | 5.807 | -3.615 | 1.00 | 0.00 C |
| ATOM | 919 | О | ARG A | 67162.370 | 6.853 | -4.062 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67160.158 | 5.956 | -5.408 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67158.907 | 5.359 | -6.030 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67158.567 | 6.031 | -7.350 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67157.502 | 5.330 | -8.063 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67157.666 | 4.161 | -8.677 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67158.849 | 3.558 | -8.668 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67156.644 | 3.591 | -9.302 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.719 | 3.493 | -3.465 | 1.00 | 0.00 H |
| ATOM | 928 | НА | ARG A | 67161.311 | 4.220 | -4.917 | 1.00 | 0.00 H |
| ATOM | 929 | 1HB | ARG A | 67159.886 | 6.877 | -4.916 | 1.00 | 0.00 H |
| ATOM | 930 2 | 2HB | ARG A | 67160.859 | 6.174 | -6.199 | 1.00 | 0.00 H |
| ATOM | 931 | 1HG | ARG A | 67159.071 | 4.306 | -6.206 | 1.00 | 0.00 H |
| ATOM | 932 | 2HG | ARG A | 67158.080 | 5.488 | -5.346 | 1.00 | 0.00 H |
| ATOM | 933 | 1HD | ARG A | 67158.248 | 7.043 | -7.152 | 1.00 | 0.00 H |

| ATOM | 934 2 | 2HD | ARG A | 67159.452 | 6.048 | -7.969 | 1.00 | 0.00 H |
|------|-------|--------|-------|-----------|--------|--------|------|--------|
| ATOM | 935 | HE | ARG A | 67156.618 | 5.753 | -8.086 | 1.00 | 0.00 H |
| ATOM | 936 1 | HH1. | ARG A | 67159.623 | 3.982 | -8.199 | 1.00 | 0.00 H |
| ATOM | 937 2 | 2HH1. | ARG A | 67158.966 | 2.679 | -9.131 | 1.00 | 0.00 H |
| ATOM | 938 1 | HH2 | ARG A | 67155.752 | 4.040 | -9.312 | 1.00 | 0.00 H |
| ATOM | 939 2 | 2HH2 . | ARG A | 67156.767 | 2.712 | -9.763 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.269 | 5.284 | -2.451 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.274 | 5.938 | -1.632 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.724 | 7.136 | -0.883 | 1.00 | 0.00 C |
| ATOM | 943 | O | GLY A | 68163.458 | 8.076 | -0.580 | 1.00 | O.00 O |
| ATOM | 944 | Н | GLY A | 68161.859 | 4.449 | -2.145 | 1.00 | 0.00 H |
| ATOM | 945 1 | HA | GLY A | 68163.658 | 5.225 | -0.917 | 1.00 | 0.00 H |
| ATOM | 946 2 | 2HA | GLY A | 68164.084 | 6.265 | -2.268 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.430 | 7.102 | -0.584 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.783 | 8.193 | 0.133 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69159.899 | 7.658 | 1.256 | 1.00 | 0.00 C |
| ATOM | 950 | О | THR A | 69158.746 | 7.291 | 1.030 | 1.00 | 0.00 O |
| ATOM | 951 | CB | THR A | 69159.948 | 9.040 | -0.828 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.661 | 9.285 | -2.028 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69159.546 | 10.380 | -0.251 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.897 | 6.324 | -0.852 | 1.00 | 0.00 H |
| ATOM | 955 | НА | THR A | 69161.556 | 8.811 | 0.565 | 1.00 | 0.00 H |
| ATOM | 956 | HB | THR A | 69159.044 | 8.501 | -1.074 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69160.425 | 8.623 | -2.681 | 1.00 | 0.00 H |
| ATOM | 958 | HG2 | THR A | 69159.640 | 11.143 | -1.010 | 1.00 | 0.00 H |
| ATOM | 959 2 | 2HG2 | THR A | 69160.189 | 10.619 | 0.583 | 1.00 | 0.00 H |
| ATOM | 960 3 | 3HG2 | THR A | 69158.521 | 10.334 | 0.087 | 1.00 | 0.00 H |

| ATOM | 961 | N | ARG A | 70160.448 | 7.616 | 2.465 | 1.00 | 0.00 N | |
|------|-------|------|-------|------------|-------|--------|------|--------|--|
| ATOM | 962 | CA | ARG A | 70159.709 | 7.125 | 3.623 | 1.00 | 0.00 C | |
| ATOM | 963 | C | ARG A | 70158.552 | 8.058 | 3.966 | 1.00 | 0.00 C | |
| ATOM | 964 | O | ARG A | 70158.739 | 9.263 | 4.126 | 1.00 | 0.00 O | |
| ATOM | 965 | СВ | ARG A | 70160.641 | 6.985 | 4.828 | 1.00 | 0.00 C | |
| ATOM | 966 | CG | ARG A | 70159.945 | 6.478 | 6.082 | 1.00 | 0.00 C | |
| ATOM | 967 | CD | ARG A | 70159.718 | 7.595 | 7.090 | 1.00 | 0.00 C | |
| ATOM | 968 | NE | ARG A | 70160.355 | 7.311 | 8.373 | 1.00 | 0.00 N | |
| ATOM | 969 | CZ | ARG A | 70161.654 | 7.482 | 8.610 | 1.00 | 0.00 C | |
| ATOM | 970 | NH1 | ARG A | 70162.457 | 7.933 | 7.653 | 1.00 | 0.00 N | |
| ATOM | 971 | NH2 | ARG A | 70162.152 | 7.201 | 9.806 | 1.00 | 0.00 N | |
| ATOM | 972 | Н | ARG A | 70161.371 | 7.922 | 2.583 | 1.00 | 0.00 H | |
| ATOM | 973 | НА | ARG A | 70159.310 | 6.153 | 3.374 | 1.00 | 0.00 H | |
| ATOM | 974 | lНВ | ARG A | 70161.433 | 6.293 | 4.577 | 1.00 | 0.00 H | |
| ATOM | 975 2 | 2HB | ARG A | 70161.075 | 7.949 | 5.046 | 1.00 | 0.00 H | |
| ATOM | 976 | IHG | ARG A | 70158.990 | 6.057 | 5.806 | 1.00 | 0.00 H | |
| ATOM | 977 2 | 2HG | ARG A | 70160.558 | 5.714 | 6.537 | 1.00 | 0.00 H | |
| ATOM | 978 | IHD | ARG A | 70160.124 | 8.513 | 6.692 | 1.00 | 0.00 H | |
| ATOM | 979 2 | 2HD | ARG A | 70158.654 | 7.709 | 7.245 | 1.00 | 0.00 H | |
| ATOM | 980 | HE | ARG A | 70159.786 | 6.977 | 9.097 | 1.00 | 0.00 H | |
| ATOM | 981 | IHH1 | ARG A | 70162.087 | 8.147 | 6.749 | 1.00 | 0.00 H | |
| ATOM | 982 | 2HH1 | ARG A | 70163.431 | 8.058 | 7.838 | 1.00 | 0.00 H | |
| ATOM | 983 | 1HH2 | ARG A | 70161.552 | 6.861 | 10.530 | 1.00 | 0.00 H | |
| ATOM | 984 2 | 2HH2 | ARG A | 70163.127 | 7.329 | 9.983 | 1.00 | 0.00 H | |
| ATOM | 985 | N | TYR A | 71.157.355 | 7.490 | 4.077 | 1.00 | 0.00 N | |
| ATOM | 986 | CA | TYR A | 71156.166 | 8.269 | 4.402 | 1.00 | 0.00 C | |
| ATOM | 987 | C | TYR A | 71155.674 | 7.950 | 5.809 | 1.00 | 0.00 C | |

| ATOM | 988 | Ο | TYR A | 71155.102 | 8.804 | 6.486 | 1.00 | 0.00 O |
|--------|------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 989 | CB | TYR A | 71155.057 | 7.991 | 3.386 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.312 | 8.601 | 2.026 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.252 | 7.827 | 0.874 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.614 | 9.951 | 1.894 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.486 | 8.380 | -0.370 | 1.00 | 0.00 C |
| ATOM - | 994 | CE2 | TYR A | 71155.847 | 10.512 | 0.653 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.783 | 9.722 | -0.476 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71156.016 | 10.276 | -1.713 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.270 | 6.524 | 3.937 | 1.00 | 0.00 H |
| ATOM | 998 | HA | TYR A | 71156.431 | 9.314 | 4.354 | 1.00 | 0.00 H |
| ATOM | 999 | 1HB | TYR A | 71154.956 | 6.924 | 3.256 | 1.00 | 0.00 H |
| ATOM | 1000 | 2HB | TYR A | 71154.126 | 8.393 | 3.761 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.020 | 6.775 | 0.960 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.664 | 10.567 | 2.780 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.435 | 7.761 | -1.254 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71156.080 | 11.563 | 0.571 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71156.854 | 9.955 | -2.056 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72155.900 | 6.714 | 6.244 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.480 | 6.283 | 7.572 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.457 | 5.262 | 8.147 | 1.00 | 0.00 C |
| ATOM | 1009 | О | PHE A | 72157.463 | 4.930 | 7.521 | 1.00 | 0.00 O |
| ATOM | 1010 | CB | PHE A | 72154.074 | 5.683 | 7.515 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72153.907 | 4.646 | 6.442 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72153.991 | 3.296 | 6.745 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72153.664 | 5.020 | 5.130 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72153.838 | 2.340 | 5.760 | 1.00 | 0.00 C |

| ATOM | 1015 | CE2 | PHE A | 72153.510 | 4.068 | 4.140 | 1.00 | 0.00 C | |
|------|--------|------------|-------|-----------|-------|--------|------|--------|---|
| ATOM | 1016 | CZ | PHE A | 72153.597 | 2.726 | 4.456 | 1.00 | 0.00 C | |
| ATOM | 1017 | Н | PHE A | 72156.362 | 6.078 | 5.659 | 1.00 | 0.00 H | |
| ATOM | 1018 | HA | PHE A | 72155.466 | 7.150 | 8.214 | 1.00 | 0.00 H | |
| ATOM | 1019 1 | НВ | PHE A | 72153.850 | 5.219 | 8.463 | 1.00 | 0.00 H | |
| ATOM | 1020 2 | :HB | PHE A | 72153.361 | 6.474 | 7.328 | 1.00 | 0.00 H | |
| ATOM | 1021 | HD1 | PHE A | 72154.180 | 2.993 | 7.765 | 1.00 | 0.00 H | |
| ATOM | 1022 | HD2 | PHE A | 72153.597 | 6.069 | 4.882 | 1.00 | 0.00 H | |
| ATOM | 1023 | HE1 | PHE A | 72153.906 | 1.291 | 6.009 | 1.00 | 0.00 H | |
| ATOM | 1024 | HE2 | PHE A | 72153.321 | 4.372 | 3.121 | 1.00 | 0.00 H | |
| ATOM | 1025 | HZ | PHE A | 72153.476 | 1.980 | 3.684 | 1.00 | 0.00 H | |
| ATOM | 1026 | N | THR A | 73156.152 | 4.768 | 9.342 | 1.00 | 0.00 N | |
| ATOM | 1027 | CA | THR A | 73157.003 | 3.784 | 10.003 | 1.00 | 0.00 C | |
| ATOM | 1028 | C . | THR A | 73156.260 | 2.467 | 10.201 | 1.00 | 0.00 C | |
| ATOM | 1029 | O | THR A | 73155.275 | 2.404 | 10.938 | 1.00 | 0.00 O | |
| ATOM | 1030 | CB | THR A | 73157.485 | 4.319 | 11.352 | 1.00 | 0.00 C | ٠ |
| ATOM | 1031 | OG1 | THR A | 73157.819 | 5.693 | 11.256 | 1.00 | 0.00 O | |
| ATOM | 1032 | CG2 | THR A | 73158.697 | 3.588 | 11.888 | 1.00 | 0.00 C | |
| ATOM | 1033 | Н | THR A | 73155.336 | 5.071 | 9.791 | 1.00 | 0.00 H | |
| ATOM | 1034 | НА | THR A | 73157.860 | 3.608 | 9.369 | 1.00 | 0.00 H | |
| ATOM | 1035 | НВ | THR A | 73156.689 | 4.214 | 12.075 | 1.00 | 0.00 H | |
| ATOM | 1036 | HG1 | THR A | 73157.943 | 6.054 | 12.137 | 1.00 | 0.00 H | |
| ATOM | 1037 1 | HG2 | THR A | 73158.608 | 3.479 | 12.959 | 1.00 | 0.00 H | |
| ATOM | 1038 2 | HG2 | THR A | 73159.589 | 4.151 | 11.656 | 1.00 | 0.00 H | |
| ATOM | 1039 3 | HG2 | THR A | 73158.759 | 2.610 | 11.431 | 1.00 | 0.00 H | |
| ATOM | 1040 | N | CYS A | 74156.736 | 1.418 | 9.539 | 1.00 | 0.00 N | |
| ATOM | 1041 | CA | CYS A | 74156.116 | 0.102 | 9.643 | 1.00 | 0.00 C | |

| ATOM | 1042 | C | CYS A | 74157.174 | -0.992 | 9.725 | 1.00 | 0.00 C | |
|------|--------|-----|-------|-----------|---------|--------|------|--------|---|
| ATOM | 1043 | O | CYS A | 74158.373 | -0.717 | 9.671 | 1.00 | 0.00 O | |
| ATOM | 1044 | СВ | CYS A | 74155.198 | - 0.148 | 8.444 | 1.00 | 0.00 C | |
| ATOM | 1045 | SG | CYS A | 74153.512 | 0.467 | 8.665 | 1.00 | 0.00 S | |
| ATOM | 1046 | Н | CYS A | 74157.524 | 1.531 | 8.967 | 1.00 | 0.00 H | |
| ATOM | 1047 | ΗA | CYSA | 74155.525 | 0.085 | 10.546 | 1.00 | 0.00 H | |
| ATOM | 1048 | IНВ | CYS A | 74155.613 | 0.339 | 7.575 | 1.00 | 0.00 H | |
| ATOM | 1049 2 | 2HB | CYS A | 74155.140 | -1.211 | 8.261 | 1.00 | 0.00 H | |
| ATOM | 1050 | HG | CYS A | 74153.269 | 0.955 | 7.875 | 1.00 | 0.00 H | |
| ATOM | 1051 | N | ALA A | 75156.723 | -2.236 | 9.856 | 1.00 | 0.00 N | |
| ATOM | 1052 | CA | ALA A | 75157.631 | -3.373 | 9.946 | 1.00 | 0.00 C | |
| ATOM | 1053 | C | ALA A | 75158.416 | -3.552 | 8.652 | 1.00 | 0.00 C | |
| ATOM | 1054 | O | ALA A | 75158.263 | -2.776 | 7.708 | 1.00 | 0.00 O | |
| ATOM | 1055 | СВ | ALAA | 75156.857 | -4.640 | 10.276 | 1.00 | 0.00 C | |
| ATOM | 1056 | Η. | ALA A | 75155.756 | -2.393 | 9.894 | 1.00 | 0.00 H | |
| ATOM | 1057 | НА | ALA A | 75158.325 | -3.183 | 10.752 | 1.00 | 0.00 H | - |
| ATOM | 1058 | lНВ | ALA A | 75156.841 | -4.784 | 11.347 | 1.00 | 0.00 H | |
| ATOM | 1059 2 | 2HB | ALA A | 75157.337 | -5.487 | 9.807 | 1.00 | 0.00 H | |
| ATOM | 1060 3 | ЗНВ | ALA A | 75155.846 | -4.551 | 9.910 | 1.00 | 0.00 H | |
| ATOM | 1061 | N | LEU A | 76159.258 | -4.580 | 8,613 | 1.00 | 0.00 N | |
| ATOM | 1062 | CA | LEU A | 76160.068 | -4.861 | 7.434 | 1.00 | 0.00 C | |
| ATOM | 1063 | C | LEU A | 76159.357 | -5.842 | 6.507 | 1.00 | 0.00 C | |
| ATOM | 1064 | O | LEU A | 76158.756 | -6.816 | 6.960 | 1.00 | 0.00 O | |
| ATOM | 1065 | CB | LEU A | 76161.428 | -5.427 | 7.847 | 1.00 | 0.00 C | |
| ATOM | 1066 | CG | LEU A | 76162.316 | -4.465 | 8.637 | 1.00 | 0.00 C | |
| ATOM | 1067 | CD1 | LEU A | 76163.393 | -5.228 | 9.391 | 1.00 | 0.00 C | |
| ATOM | 1068 | CD2 | LEU A | 76162.943 | -3.436 | 7.708 | 1.00 | 0.00 C | |

| ATOM | 1069 | Н | LEU A | 76159.336 | -5.163 | 9.397 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1070 | HA | LEU A | 76160.219 | -3.931 | 6.908 | 1.00 | 0.00 H |
| ATOM | 1071 | 1HB | LEU A | 76161.259 | -6.307 | 8.451 | 1.00 | 0.00 H |
| ATOM | 1072 | 2HB | LEU A | 76161.959 | -5.720 | 6.954 | 1.00 | 0.00 H |
| ATOM | 1073 | HG | LEU A | 76161.711 | -3.938 | 9.361 | 1.00 | 0.00 H |
| ATOM | 1074 | 1HD1 | LEU A | 76164.253 | -4.593 | 9.534 | 1.00 | 0.00 H |
| ATOM | 1075 | 2HD1 | LEU A | 76163.679 | -6.102 | 8.824 | 1.00 | 0.00 H |
| ATOM | 1076 | 3HD1 | LEU A | 76163.009 | -5.535 | 10.354 | 1.00 | 0.00 H |
| ATOM | 1077 | 1HD2 | LEU A | 76163.039 | -3.855 | 6.717 | 1.00 | 0.00 H |
| ATOM | 1078 | 2HD2 | LEU A | 76163.920 | -3.162 | 8.079 | 1.00 | 0.00 H |
| ATOM | 1079 | 3HD2 | LEU A | 76162.315 | -2.558 | 7.666 | 1.00 | 0.00 H |
| ATOM | 1080 | N | LYS A | 77159.429 | -5.577 | 5.207 | 1.00 | 0.00 N |
| ATOM | 1081 | CA | LYS A | 77158.793 | -6.436 | 4.214 | 1.00 | 0.00 C |
| ATOM | 1082 | C | LYS A | 77157.283 | -6.478 | 4.419 | 1.00 | 0.00 C |
| ATOM | 1083 | Ο | LYS A | 77156.656 | -7.529 | 4.285 | 1.00 | 0.00 O |
| ATOM | 1084 | CB | LYS A | 77159.370 | -7.851 | 4.288 | 1.00 | 0.00 C |
| ATOM | 1085 | CG | LYS A | 77160.884 | -7.899 | 4.152 | 1.00 | 0.00 C |
| ATOM | 1086 | CD | LYS A | 77161.333 | -7.461 | 2.766 | 1.00 | 0.00 C |
| ATOM | 1087 | CE | LYS A | 77162.582 | -6.598 | 2.832 | 1.00 | 0.00 C |
| ATOM | 1088 | NZ | LYS A | 77162.254 | -5.158 | 3.023 | 1.00 | 0.00 N |
| ATOM | 1089 | Н | LYS A | 77159.924 | -4.785 | 4.906 | 1.00 | 0.00 H |
| ATOM | 1090 | HA | LYSA | 77159.001 | -6.024 | 3.238 | 1.00 | 0.00 H |
| ATOM | 1091 | 1HB | LYS A | 77159.103 | -8.287 | 5.239 | 1.00 | 0.00 H |
| ATOM | 1092 | 2HB | LYS A | 77158.940 | -8.445 | 3.496 | 1.00 | 0.00 H |
| ATOM | 1093 | 1HG | LYS A | 77161.323 | -7.240 | 4.887 | 1.00 | 0.00 H |
| ATOM | 1094 | 2HG | LYS A | 77161.220 | -8.910 | 4.327 | 1.00 | 0.00 H |
| ATOM | 1095 | 1HD | LYS A | 77161.545 | -8.337 | 2.174 | 1.00 | 0.00 H |

| ATOM | 1096 | 2HD | LYS A | 77160.538 | -6.894 | 2.304 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1097 | 1HE | LYS A | 77163.191 | -6.930 | 3.660 | 1.00 | 0.00 H |
| ATOM | 1098 2 | 2HE | LYS A | 77163.134 | -6.714 | 1.912 | 1.00 | 0.00 H |
| ATOM | 1099 | 1HZ | LYSA | 77161.291 | -4.963 | 2.679 | 1.00 | 0.00 H |
| ATOM | 1100 2 | 2HZ | LYS A | 77162.925 | -4.564 | 2.495 | 1.00 | 0.00 H |
| ATOM | 1101 3 | BHZ | LYS A | 77162.307 | -4.909 | 4.032 | 1.00 | 0.00 H |
| ATOM | 1102 | N | LYS A | 78156.702 | -5.327 | 4.745 | 1.00 | 0.00 N |
| ATOM | 1103 | CA | LYS A | 78155.265 | -5.233 | 4.968 | 1.00 | 0.00 C |
| ATOM | 1104 | C | LYS A | 78154.741 | -3.857 | 4.567 | 1.00 | 0.00 C |
| ATOM | 1105 | O | LYS A | 78153.838 | -3.316 | 5.206 | 1.00 | 0.00 O |
| ATOM | 1106 | СВ | LYS A | 78154.936 | -5.509 | 6.436 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.439 | -6.856 | 6.930 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78155.044 | -7.103 | 8.377 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYS A | 78153.565 | -7.429 | 8.503 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78153.262 | -8.159 | 9.765 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.254 | -4.523 | 4.837 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.785 | -5.980 | 4.355 | 1.00 | 0.00 H |
| ATOM | 1113 | lНВ | LYS A | 78155.384 | -4.737 | 7.045 | 1.00 | 0.00 H |
| ATOM | 11142 | 2HB | LYS A | 78153.864 | -5.480 | 6.566 | 1.00 | 0.00 H |
| ATOM | 1115 | IHG | LYS A | 78155.015 | -7.635 | 6.314 | 1.00 | 0.00 H |
| ATOM | 11162 | 2ḤG | LYS A | 78156.516 | -6.878 | 6.851 | 1.00 | 0.00 H |
| ATOM | 1117 | HD | LYS A | 78155.619 | -7.932 | 8.760 | 1.00 | 0.00 H |
| ATOM | 11182 | 2HD | LYS A | 78155.259 | -6.215 | 8.954 | 1.00 | 0.00 H |
| ATOM | 1119 | 1HE | LYS A | 78153.003 | -6.507 | 8.487 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYS A | 78153.271 | -8.042 | 7.663 | 1.00 | 0.00 H |
| ATOM | 1121 | 1HZ | LYS A | 78153.299 | -9.186 | 9.602 | 1.00 | 0.00 H |
| ATOM | 1122 | 2HZ | LYS A | 78152.312 | -7.907 | 10.105 | 1.00 | 0.00 H |

| ATOM | 1123 | 3HZ | LYS A | 78153.957 | -7.909 | 10.497 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1124 | N | ALA A | 79155.313 | -3.298 | 3.507 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.904 | -1.986 | 3.022 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.827 | -1.964 | 1.499 | 1.00 | 0.00 C |
| ATOM | 1127 | О | ALA A | 79155.846 | -1.846 | 0.817 | 1.00 | 0.00 O |
| ATOM | 1128 | СВ | ALA A | 79155.864 | -0.916 | 3.519 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79156.028 | -3.779 | 3.040 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.924 | -1.772 | 3.425 | 1.00 | 0.00 H |
| ATOM | 1131 | 1HB | ALA A | 79156.388 | -1.279 | 4.391 | 1.00 | 0.00 H |
| ATOM | 1132 | 2HB | ALA A | 79155.310 | -0.026 | 3.776 | 1.00 | 0.00 H |
| ATOM | 1133 | 3HB | ALA A | 79156.578 | -0.684 | 2.741 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.612 | -2.077 | 0.970 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.402 | -2.069 | -0.473 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.484 | -0.924 | -0.884 | 1.00 | 0.00 C |
| ATOM | 1137 | O | LEU A | 80151.354 | -0.818 | -0.407 | 1.00 | 0.00 O |
| ATOM | 1138 | CB | LEU A | 80152.808 | -3.404 | -0.928 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.489 | -3.494 | -2.422 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.744 | -3.825 | -3.216 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80151.407 | -4.534 | -2.673 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.839 | -2.167 | 1.566 | 1.00 | 0.00 H |
| ATOM | 1143 | HA | LEU A | 80154.362 | -1.934 | -0.947 | 1.00 | 0.00 H |
| ATOM | 1144 | 1HB | LEU A | 80153.508 | -4.189 | -0.682 | 1.00 | 0.00 H |
| ATOM | 1145 | 2HB | LEU A | 80151.894 | -3.573 | -0.378 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80152.122 | -2.537 | -2.764 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | LEU A | 80153.968 | -4.877 | -3.113 | 1.00 | 0.00 H |
| ATOM | 1148 | 2HD1 | LEU A | 80154.572 | -3.243 | -2.839 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80153.582 | -3.590 | -4.257 | 1.00 | 0.00 H |

| ATOM | 1150 | HD2 | LEU [·] A | 80150.440 | -4.054 | -2.672 | 1.00 | 0.00 H |
|------|--------|------|--------------------|-----------|--------|---------|------|--------|
| ATOM | 1151 2 | 2HD2 | LEU A | 80151.440 | -5.282 | -1.895 | 1.00 | 0.00 H |
| ATOM | 1152 3 | 3HD2 | LEU A | 80151.575 | -5.003 | -3.631 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.977 | -0.065 | -1.770 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.201 | 1.074 | -2.245 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.396 | 0.705 | -3.487 | 1.00 | 0.00 C |
| ATOM | 1156 | О | PHE A | 81151.813 | -0.141 | -4.280 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.123 | 2.254 | -2.554 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.759 | 2.855 | -1.332 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81153.219 | 3.986 | -0.740 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81154.894 | 2.288 | -0.775 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81153.801 | 4.540 | 0.385 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81155.479 | 2.838 | 0.349 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81154.932 | 3.966 | 0.930 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.885 | -0.201 | -2.114 | 1.00 | 0.00 H |
| ATOM | 1165 | НА | PHE A | 81151.517 | 1.359 | -1.460 | 1.00 | 0.00 H |
| ATOM | 1166 | НВ | PHE A | 81153.914 | 1.922 | -3.209 | 1.00 | 0.00 H |
| ATOM | 1167 2 | 2HB | PHE A | 81152.554 | 3.027 | -3.048 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81152.335 | 4.436 | - 1.166 | 1.00 | 0.00 H |
| ATOM | 1169 | HD2 | PHE A | 81155.323 | 1.406 | -1.228 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81153.371 | 5.423 | 0.835 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81156.364 | 2.387 | 0.773 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.389 | 4.398 | 1.808 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.242 | 1.343 | -3.650 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VAL A | 82149.380 | 1.081 | -4.796 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VALA | 82148.465 | 2.268 | -5.077 | 1.00 | 0.00 C |
| ATOM | 1176 | O | VAL A | 82148.334 | 3.174 | -4.253 | 1.00 | 0.00 O |

| ATOM | 1177 | CB | VAL A | 82148.517 | -0.175 | -4.574 | 1.00 | 0.00 C | |
|------|------|------|-------|-----------|--------|---------|------|--------|--|
| ATOM | 1178 | CG1 | VAL A | 82149.388 | -1.419 | -4.519 | 1.00 | 0.00 C | |
| ATOM | 1179 | CG2 | VALA | 82147.691 | -0.038 | -3.304 | 1.00 | 0.00 C | |
| ATOM | 1180 | Н | VAL A | 82149.965 | 2.006 | -2.984 | 1.00 | 0.00 H | |
| ATOM | 1181 | HA | VAL A | 82150.010 | 0.912 | -5.656 | 1.00 | 0.00 H | |
| ATOM | 1182 | HB | VAL A | 82147.839 | -0.273 | -5.409 | 1.00 | 0.00 H | |
| ATOM | 1183 | 1HG1 | VAL A | 82150.172 | -1.344 | -5.260 | 1.00 | 0.00 H | |
| ATOM | 1184 | 2HG1 | VAL A | 82148.784 | -2.291 | -4.723 | 1.00 | 0.00 H | |
| ATOM | 1185 | 3HG1 | VAL A | 82149.829 | -1.508 | -3.538 | 1.00 | 0.00 H | |
| ATOM | 1186 | 1HG2 | VAL A | 82146.737 | -0.526 | -3.441 | 1.00 | 0.00 H | |
| ATOM | 1187 | 2HG2 | VAL A | 82147.531 | 1.009 | -3.090 | 1.00 | 0.00 H | |
| ATOM | 1188 | 3HG2 | VAL A | 82148.217 | -0.497 | -2.480 | 1.00 | 0.00 H | |
| ATOM | 1189 | N | LYS A | 83147.834 | 2.257 | -6.247 | 1.00 | 0.00 N | |
| ATOM | 1190 | CA | LYS A | 83146.931 | 3.333 | -6.639 | 1.00 | 0.00 C | |
| ATOM | 1191 | C | LYS A | 83145.672 | 3.327 | -5.778 | 1.00 | 0.00 C | |
| ATOM | 1192 | О | LYS A | 83144.950 | 2.332 | -5.724 | 1.00 | 0.00 O | |
| ATOM | 1193 | СВ | LYS A | 83146.554 | 3.198 | -8.116 | 1.00 | 0.00 C | |
| ATOM | 1194 | CG | LYS A | 83147.716 | 3.442 | -9.064 | 1.00 | 0.00 C | |
| ATOM | 1195 | CD | LYS A | 83147.351 | 3.082 | -10.495 | 1.00 | 0.00 C | |
| ATOM | 1196 | CE | LYS A | 83147.951 | 4.066 | -11.487 | 1.00 | 0.00 C | |
| ATOM | 1197 | NZ | LYS A | 83148.395 | 3.393 | -12.739 | 1.00 | 0.00 N | |
| ATOM | 1198 | Н | LYS A | 83147.979 | 1.508 | -6.862 | 1.00 | 0.00 H | |
| ATOM | 1199 | HA | LYS A | 83147.446 | 4.270 | -6.492 | 1.00 | 0.00 H | |
| ATOM | 1200 | 1HB | LYS A | 83146.178 | 2.201 | -8.289 | 1.00 | 0.00 H | |
| ATOM | 1201 | 2HB | LYS A | 83145.776 | 3.912 | -8.343 | 1.00 | 0.00 H | |
| ATOM | 1202 | 1HG | LYS A | 83147.988 | 4.486 | -9.024 | 1.00 | 0.00 H | |
| ATOM | 1203 | 2HG | LYS A | 83148.555 | 2.837 | -8.753 | 1.00 | 0.00 H | |

1204 1HD LYS A 83147.725 2.094 -10.715 1.00 0.00 H**ATOM** LYS A 83146.276 3.093 -10.596 1.00 -0.00 H **ATOM** 1205 2HD LYS A 83147.206 4.809 -11.733 1.00 0.00 H **ATOM** 1206 1HE LYS A 83148.800 4.549 -11.027 1.00 0.00 H **ATOM** 1207 2HE **ATOM** 1208 1HZ LYS A 83148.832 2.476 -12.515 1.00 0.00 HLYS A 83149.090 3.984 -13.235 1.00 0.00 H **ATOM** 1209 2HZ 1210 3HZ LYS A 83147.580 3.233 -13.366 1.00 0.00 H**ATOM** 1211 N LEU A 84145.417 4.445 -5.109 1.00 0.00 N **ATOM** -4.250 CA LEUA 84144.246 1.00 0.00 C **ATOM** 1212 4.573 LEU A 84142.961 -5.049 1.00 0.00 C **ATOM** 1213 C 4.378 **ATOM** 1214 O LEU A 84141.971 3.858 -4.535 1.00 0.00 O LEU A 84144.237 5.944 -3.5711.00 0.00 C **ATOM** 1215 CBCG LEUA 84142.996 6.246 -2.730 1.00 0.00 C **ATOM** 1216 1.00 0.00 C -1.392 CD1 LEU A 84143.069 5.526 **ATOM** 1217 1.00 0.00 C CD2 LEU A 84142.846 7.745 -2.522**ATOM** 1218 **ATOM** 1219 Η LEU A 84146.031 5.204 -5.195 1.00 0.00 H **ATOM** 1220 HA LEUA 84144.305 3.805 -3.493 1.00 0.00 H 1.00 0.00 H LEU A 84145.105 6.008 -2.929 **ATOM** 1221 1HB 1.00 0.00 H **ATOM** 1222 2HB LEU A 84144.320 6.701 -4.335 -3.253 1.00 0.00 H 1223 HG LEUA 84142.120 5.890 **ATOM** 1224 1HD1 LEU A 84143.969 5.817 -0.874 1.00 0.00 H **ATOM** -1.559 1.00 0.00 H 1225 2HD1 LEU A 84143.079 4.458 **ATOM** 1226 3HD1 LEU A 84142.208 5.788 -0.795 1.00 0.00 H **ATOM** 0.00 H 1227 1HD2 LEU A 84143.594 8.088 -1.824 1.00 **ATOM** 1.00 0.00 H 7.959 -2.1301228 2HD2 LEU A 84141.862 **ATOM** -3.466 1.00 0.00 H 1229 3HD2 LEU A 84142.974 8.254 **ATOM** 0.00 N 4.799 -6.310 1.00 **ATOM** 1230 N LYS A 85142.985

| ATOM | 1231 | CA | LYS A | 85141.821 | 4.669 | -7.179 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|---------|----------------|------|--------|
| ATOM | 1232 | C | LYS A | 85141.476 | 3.201 | -7.415 | 1.00 | 0.00 C |
| ATOM | 1233 | O | LYS A | 85140.323 | 2.860 | -7.676 | 1.00 | 0.00 O |
| ATOM | 1234 | СВ | LYS A | 85142.078 | 5.366 | -8.517 | 1.00 | 0.00 C |
| ATOM | 1235 | CG | LYS A | 85143.400 | 4.979 | - 9.161 | 1.00 | 0.00 C |
| ATOM | 1236 | CD | LYS A | 85144.399 | 6.124 | -9.118 | 1.00 | 0.00 C |
| ATOM | 1237 | CE | LYS A | 85144.251 | 7.037 - | 10.325 | 1.00 | 0.00 C |
| ATOM | 1238 | NZ | LYS A | 85144.698 | 8.426 - | 10.028 | 1.00 | 0.00 N |
| ATOM | 1239 | Н | LYS A | 85143.802 | 5.205 | -6.663 | 1.00 | 0.00 H |
| ATOM | 1240 | НА | LYS A | 85140.987 | 5.149 | -6.689 | 1.00 | 0.00 H |
| ATOM | 1241 | lНВ | LYS A | 85141.281 | 5.111 | -9.201 | 1.00 | 0.00 H |
| ATOM | 1242 2 | 2HB | LYS A | 85142.077 | 6.434 | -8.360 | 1.00 | 0.00 H |
| ATOM | 1243 | НG | LYS A | 85143.814 | 4.134 | -8.631 | 1.00 | 0.00 H |
| ATOM | 1244 2 | 2HG | LYS A | 85143.222 | 4.706 - | 10.191 | 1.00 | 0.00 H |
| ATOM | 1245 | IHD | LYS A | 85144.235 | 6.700 | -8.221 | 1.00 | 0.00 H |
| ATOM | 1246 2 | 2HD | LYS A | 85145.399 | 5.715 | -9.109 | 1.00 | 0.00 H |
| ATOM | 1247 | HE | LYS A | 85144.847 | 6.643 - | 11.134 | 1.00 | 0.00 H |
| ATOM | 1248 2 | 2HE | LYS A | 85143.212 | 7.057 - | 10.619 | 1.00 | 0.00 H |
| ATOM | 1249 | ΙHΖ | LYS A | 85144.700 | 8.995 - | 10.899 | 1.00 | 0.00 H |
| ATOM | 1250 2 | 2HZ | LYS A | 85145.659 | 8.416 | -9.632 | 1.00 | 0.00 H |
| ATOM | 1251 3 | BHZ | LYS A | 85144.056 | 8.868 | -9.338 | 1.00 | 0.00 H |
| ATOM | 1252 | N | SER A | 86142.483 | 2.338 | -7.322 | 1.00 | 0.00 N |
| ATOM | 1253 | CA | SER A | 86142.283 | 0.908 | -7.525 | 1.00 | 0.00 C |
| ATOM | 1254 | C | SER A | 86142.180 | 0.177 | -6.191 | 1.00 | 0.00 C |
| ATOM | 1255 | O | SER A | 86142.582 | -0.981 | -6.073 | 1.00 | 0.00 O |
| ATOM | 1256 | СВ | SER A | 86143.430 | 0.324 | -8.352 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.578 | 1.016 | -9.581 | 1.00 | 0.00 O |

| ATOM | 1258 | Н | SER A | 86143.380 | 2.669 | -7.111 | 1.00 | 0.00 H |
|------|--------|-----|---------|-----------|--------|--------|------|--------|
| ATOM | 1259 | НА | SER A | 86141.358 | 0.777 | -8.067 | 1.00 | 0.00 H |
| ATOM | 1260 | lНВ | SER A | 86144.351 | 0.407 | -7.794 | 1.00 | 0.00 H |
| ATOM | 1261 2 | 2HB | SER A | 86143.228 | -0.716 | -8.561 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86142.715 | 1.148 | -9.979 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.639 | 0.860 | -5.188 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.482 | 0.275 | -3.861 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87140.008 | 0.152 | -3.491 | 1.00 | 0.00 C |
| ATOM | 1266 | О | CYS A | 87139.153 | 0.819 | -4.073 | 1.00 | 0.00 O |
| ATOM | 1267 | СВ | CYS A | 87142.211 | 1.124 | -2.818 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYSA | 87143.995 | 0.839 | -2.751 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYS A | 87141.337 | 1.779 | -5.343 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87141.920 | -0.712 | -3.878 | 1.00 | 0.00 H |
| ATOM | 1271 | lНВ | CYS A | 87142.055 | 2.168 | -3.041 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.806 | 0.906 | -1.840 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.366 | 1.082 | -3.603 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.715 | -0.707 | -2.519 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.344 | -0.918 | -2.072 | 1.00 | 0.00 C |
| ATOM | 1276 | Ç | ARG A | 88138.274 | -0.998 | -0.547 | 1.00 | 0.00 C |
| ATOM | 1277 | O | ARG A | 88139.152 | -1.577 | 0.091 | 1.00 | 0.00 O |
| ATOM | 1278 | СВ | ARG A | 88137.777 | -2.198 | -2.689 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88136.918 | -1.952 | -3.918 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.437 | -1.957 | -3.574 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88134.598 | -2.033 | -4.768 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88133.279 | -2.220 | -4.736 | 1.00 | 0.00 C |
| ATOM | 1283 | NH | ARG A | 88132.649 | -2.351 | -3.576 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | 2 ARG A | 88132.592 | -2.276 | -5.868 | 1.00 | 0.00 N |

| ATOM | 1285 | Н | ARG A | 88140.440 | -1.210 | -2.093 | 1.00 | 0.00 H |
|--------|------|-------------|-------|-----------|---------|---------|------|--------|
| ATOM | 1286 | НА | ARG A | 88137.756 | -0.077 | -2.406 | 1.00 | 0.00 H |
| ATOM | 1287 | 1 HB | ARG A | 88138.597 | -2.841 | -2.972 | 1.00 | 0.00 H |
| ATOM | 1288 | 2HB | ARG A | 88137.173 | -2.705 | -1.950 | 1.00 | 0.00 H |
| ATOM | 1289 | 1HG | ARG A | 88137.176 | -0.992 | -4.340 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88137.113 | -2.730 | -4.642 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88135.230 | -2.810 | -2.946 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.203 | -1.050 | -3.037 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88135.038 | -1.938 | -5.638 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88133.161 | -2.310 | -2.719 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88131.658 | -2.491 | -3.559 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88133.062 | -2.176 | - 6.745 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88131.601 | -2.416 | -5.845 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.224 | -0.415 | 0.060 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89137.049 | -0.428 | 1.516 | 1.00 | 0.00 C |
| ATOM . | 1300 | C | PRO A | 89137.081 | - 1.842 | 2.089 | 1.00 | 0.00 C |
| ATOM | 1301 | О | PRO A | 89136.463 | -2.756 | 1.545 | 1.00 | 0.00 O |
| ATOM | 1302 | СВ | PRO A | 89135.666 | 0.197 | 1.720 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.435 | 1.020 | 0.501 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89136.128 | 0.299 | -0.621 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.797 | 0.175 | 2.009 | 1.00 | 0.00 H |
| ATOM | 1306 | 1HB | PRO A | 89134.926 | -0.584 | 1.817 | 1.00 | 0.00 H |
| ATOM | 1307 | 2HB | PRO A | 89135.672 | 0.807 | 2.612 | 1.00 | 0.00 H |
| ATOM | 1308 | 1HG | PRO A | 89134.376 | 1.093 | 0.303 | 1.00 | 0.00 H |
| ATOM | 1309 | 2HG | PRO A | 89135.862 | 2.003 | 0.634 | 1.00 | 0.00 H |
| ATOM | 1310 | 1HD | PRO A | 89135.452 | -0.396 | -1.098 | 1.00 | 0.00 H |
| ATOM | 1311 | 2HD | PRO A | 89136.516 | 1.005 | -1.340 | 1.00 | 0.00 H |

| ATOM | 1312 | N | ASPA | 90137.806 | -2.014 | 3.189 | 1.00 | 0.00 N |
|------|--------|-----|--------|-----------|--------|--------|------|--------|
| ATOM | 1313 | CA | ASP A. | 90137.917 | -3.316 | 3.835 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASP A | 90136.972 | -3.412 | 5.029 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASPA | 90137.077 | -2.637 | 5.980 | 1.00 | 0.00 O |
| ATOM | 1316 | СВ | ASPA | 90139.356 | -3.565 | 4.287 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90139.717 | -5.038 | 4.282 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASP A | 90140.547 | -5.448 | 5.120. | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | ASP A | 90139.169 | -5.780 | 3.441 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.276 | -1.246 | 3.577 | 1.00 | 0.00 H |
| ATOM | 1321 | НА | ASPA | 90137.640 | -4.068 | 3.111 | 1.00 | 0.00 H |
| ATOM | 1322 1 | НВ | ASPA | 90140.030 | -3.047 | 3.622 | 1.00 | 0.00 H |
| ATOM | 1323 2 | 2HB | ASPA | 90139.482 | -3.185 | 5.290 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.050 | -4.367 | 4.972 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91135.087 | -4.563 | 6.049 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91135.527 | -5.694 | 6.974 | 1.00 | 0.00 C |
| ATOM | 1327 | O | SER A | 91134.698 | -6.422 | 7.519 | 1.00 | 0.00 O |
| ATOM | 1328 | CB | SER A | 91133.703 | -4.870 | 5.475 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91132.679 | -4.405 | 6.337 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91136.017 | -4.954 | 4.188 | 1.00 | 0.00 H |
| ATOM | 1331 | НА | SER A | 91135.037 | -3.649 | 6.618 | 1.00 | 0.00 H |
| ATOM | 1332 | IHB | SER A | 91133.597 | -4.383 | 4.517 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91133.595 | -5.937 | 5.350 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91131.982 | -5.063 | 6.390 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92136.837 | -5.835 | 7.146 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92137.387 | -6.876 | 8.006 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92137.020 | -6.628 | 9.465 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92136.878 | -7.568 | 10.247 | 1.00 | 0.00 O |

| ATO 3 6 | 1220 | OB | 4 D.C. 4 | 02120 000 | C 0.40 | 7.054 | 1 00 | 0.00.0 |
|---------|--------|--------|----------|-------------|---------|--------|------|--------|
| ATOM | 1339 | СВ | ARG A | 92138.909 | -6.940 | 7.854 | | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92139.365 | -7.676 | 6.605 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92139.163 | -9.177 | 6.737 | 1.00 | 0.00 C |
| ATOM | 1342 | NE | ARG A | 92137.960 | -9.631 | 6.042 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92137.717 | -10.903 | 5.736 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92138.590 - | 11.850 | 6.059 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92136.599 - | 11.230 | 5.103 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92137.449 | -5.222 | 6.686 | 1.00 | 0.00 H |
| ATOM | 1347 | НА | ARG A | 92136.964 | -7.819 | 7.695 | 1.00 | 0.00 H |
| ATOM | 1348 | 1HB | ARG A | 92139.298 | -5.934 | 7.815 | 1.00 | 0.00 H |
| ATOM | 1349 2 | 2HB | ARG A | 92139.324 | -7.444 | 8.715 | 1.00 | 0.00 H |
| ATOM | 1350 | IHG | ARG A | 92138.794 | -7.320 | 5.761 | 1.00 | 0.00 H |
| ATOM | 1351 2 | 2HG | ARG A | 92140.414 | -7.475 | 6.444 | 1.00 | 0.00 H |
| ATOM | 1352 | IHD | ARG A | 92140.021 | -9.681 | 6.317 | 1.00 | 0.00 H |
| ATOM | 1353 2 | 2HD | ARG A | 92139.078 | -9.426 | 7.785 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92137.299 | -8.953 | 5.792 | 1.00 | 0.00 H |
| ATOM | 1355 | lHH1. | ARG A | 92139.436 - | 11.610 | 6.536 | 1.00 | 0.00 H |
| ATOM | 13562 | 2HH1 . | ARG A | 92138.402 - | 12.804 | 5.826 | 1.00 | 0.00 H |
| ATOM | 1357 | HH2 | ARG A | 92135.937 - | 10.522 | 4.858 | 1.00 | 0.00 H |
| ATOM | 1358 | 2НН2 | ARG A | 92136.416 - | 12.187 | 4.873 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93136.868 | -5.358 | 9.825 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93136.517 | -4.988 | 11.192 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93135.373 | -3.979 | 11.206 | 1.00 | 0.00 C |
| ATOM | 1362 | О | PHE A | 93135.331 | -3.085 | 12.051 | 1.00 | 0.00 O |
| ATOM | 1363 | СВ | PHE A | 93137.733 | -4.406 | 11.914 | 1.00 | 0.00 C |
| ATOM | 1364 | CG | PHE A | 93138.849 | -5.395 | 12.101 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93139.524 | -5.913 | 11.008 | 1.00 | 0.00 C |
| | | | | | | | | |

| ATOM | 1366 | CD2 | PHE A | 93139.223 | -5.804 | 13.372 | 1.00 | 0.00 C |
|------|--------|------------|-------|-----------|--------|--------|------|--------|
| ATOM | 1367 | CE1 | PHE A | 93140.552 | -6.822 | 11.178 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93140.248 | -6.713 | 13.547 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ | PHE A | 93140.913 | -7.223 | 12.449 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93136.994 | -4.652 | 9.157 | 1.00 | 0.00 H |
| ATOM | 1371 | HA | PHE A | 93136.199 | -5.882 | 11.705 | 1.00 | 0.00 H |
| ATOM | 1372 | lНВ | PHE A | 93138.119 | -3.576 | 11.342 | 1.00 | 0.00 H |
| ATOM | 1373 2 | 2HB | PHE A | 93137.431 | -4.056 | 12.889 | 1.00 | 0.00 H |
| ATOM | 1374 | HD1 | PHE A | 93139.242 | -5.600 | 10.014 | 1.00 | 0.00 H |
| ATOM | 1375 | HD2 | PHE A | 93138.702 | -5.407 | 14.231 | 1.00 | 0.00 H |
| ATOM | 1376 | HE1 | PHE A | 93141.070 | -7.219 | 10.317 | 1.00 | 0.00 H |
| ATOM | 1377 | HE2 | PHE A | 93140.529 | -7.025 | 14.542 | 1.00 | 0.00 H |
| ATOM | 1378 | HZ | PHE A | 93141.716 | -7.934 | 12.584 | 1.00 | 0.00 H |
| ATOM | 1379 | N | ALA A | 94134.446 | -4.128 | 10.266 | 1.00 | 0.00 N |
| ATOM | 1380 | CA | ALA A | 94133.302 | -3.230 | 10.171 | 1.00 | 0.00 C |
| ATOM | 1381 | C | ALA A | 94132.101 | -3.789 | 10.924 | 1.00 | 0.00 C |
| ATOM | 1382 | О | ALA A | 94131.718 | -4.944 | 10.733 | 1.00 | 0.00 O |
| ATOM | 1383 | CB | ALA A | 94132.944 | -2.982 | 8.713 | 1.00 | 0.00 C |
| ATOM | 1384 | Н | ALA A | 94134.534 | -4.860 | 9.620 | 1.00 | 0.00 H |
| ATOM | 1385 | HA | ALA A | 94133.583 | -2.285 | 10.613 | 1.00 | 0.00 H |
| ATOM | 1386 | lHB | ALA A | 94132.185 | -3.686 | 8.404 | 1.00 | 0.00 H |
| ATOM | 1387 | 2HB | ALA A | 94133.824 | -3.111 | 8.100 | 1.00 | 0.00 H |
| ATOM | 1388 3 | 3HB | ALA A | 94132.570 | -1.976 | 8.600 | 1.00 | 0.00 H |
| ATOM | 1389 | N | SER A | 95131.509 | -2.964 | 11.783 | 1.00 | 0.00 N |
| ATOM | 1390 | CA | SER A | 95130.351 | -3.376 | 12.566 | 1.00 | 0.00 C |
| ATOM | 1391 | C . | SER A | 95129.056 | -3.097 | 11.811 | 1.00 | 0.00 C |
| ATOM | 1392 | O | SER A | 95128.835 | -1.988 | 11.325 | 1.00 | 0.00 O |

| ATOM | 1393 | СВ | SER A | 95130.336 | -2.652 | 13.913 | 1.00 | 0.00 C |
|------|------|------------|-------|-----------|--------|--------|------|--------|
| ATOM | 1394 | OG | SER A | 95130.569 | -1.263 | 13.749 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95131.861 | -2.056 | 11.891 | 1.00 | 0.00 H |
| ATOM | 1396 | НА | SER A | 95130.430 | -4.438 | 12.740 | 1.00 | 0.00 H |
| ATOM | 1397 | 1HB | SER A | 95129.372 | -2.788 | 14.382 | 1.00 | 0.00 H |
| ATOM | 1398 | 2HB | SER A | 95131.107 | -3.062 | 14.548 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95129.901 | -0.892 | 13.169 | 1.00 | 0.00 H |
| ATOM | 1400 | N | LEU A | 96128.201 | -4.111 | 11.717 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96126.927 | -3.976 | 11.022 | 1.00 | 0.00 C |
| ATOM | 1402 | , C | LEU A | 96125.985 | -5.119 | 11.386 | 1.00 | 0.00 C |
| ATOM | 1403 | О | LEU A | 96126.309 | -6.290 | 11,190 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96127.150 | -3.939 | 9.507 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96127.031 | -2.553 | 8.870 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96127.658 | -2.548 | 7.484 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96125.573 | -2.123 | 8.800 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96128.433 | -4.971 | 12.126 | 1.00 | 0.00 H |
| ATOM | 1409 | HA | LEU A | 96126.478 | -3.044 | 11.333 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96128.137 | -4.324 | 9.301 | 1.00 | 0.00 H |
| ATOM | 1411 | 2HB | LEU A | 96126.424 | -4.588 | 9.040 | 1.00 | 0.00 H |
| ATOM | 1412 | HG | LEU A | 96127.563 | -1.837 | 9.479 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96127.346 | -3.430 | 6.944 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96128.733 | -2.544 | 7.576 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96127.339 | -1.666 | 6.948 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96124.961 | -2.970 | 8.524 | 1.00 | 0.00 H |
| ATOM | 1417 | 2HD2 | LEU A | 96125.463 | -1.344 | 8.060 | 1.00 | 0.00 H |
| ATOM | 1418 | 3HD2 | LEU A | 96125.261 | -1.752 | 9.764 | 1.00 | 0.00 H |
| ATOM | 1419 | N | GLN A | 97124.818 | -4.770 | 11.919 | 1.00 | 0.00 N |

| ATOM | 1420 | CA | GLN A | 97123.829 | -5.767 | 12.312 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 1421 | C | GLN A | 97122.418 | -5.307 | 11.952 | 1.00 | 0.00 C |
| ATOM | 1422 | O | GLN A | 97121.781 | -4.580 | 12.715 | 1.00 | 0.00 O |
| ATOM | 1423 | СВ | GLN A | 97123.920 | -6.040 | 13.814 | 1.00 | 0.00 C |
| ATOM | 1424 | CG | GLN A | 97124.007 | -4.778 | 14.657 | 1.00 | 0.00 C |
| ATOM | 1425 | CD | GLN A | 97123.601 | -5.011 | 16.100 | 1.00 | 0.00 C |
| ATOM | 1426 | OE1 | GLN A | 97122.523 | -4.598 | 16.527 | 1.00 | 0.00 O |
| ATOM | 1427 | NE2 | GLN A | 97124.464 | -5.675 | 16.858 | 1.00 | 0.00 N |
| ATOM | 1428 | Н | GLN A | 97124.618 | - 3.821 | 12.052 | 1.00 | 0.00 H |
| ATOM | 1429 | НА | GLN A | 97124.047 | -6.679 | 11.777 | 1.00 | 0.00 H |
| ATOM | 1430 | 1HB | GLN A | 97123.045 | -6.593 | 14.122 | 1.00 | 0.00 H |
| ATOM | 1431 | 2HB | GLN A | 97124.798 | -6.637 | 14.007 | 1.00 | 0.00 H |
| ATOM | 1432 | 1HG | GLN A | 97125.024 | -4.418 | 14.640 | 1.00 | 0.00 H |
| ATOM | 1433 | 2HG | GLN A | 97123.354 | -4.030 | 14.231 | 1.00 | 0.00 H |
| ATOM | 1434 | 1HE2 | GLN A | 97125.305 | -5.974 | 16.450 | 1.00 | 0.00 H |
| ATOM | 1435 | 2HE2 | GLN A | 97124.228 | -5.840 | 17.794 | 1.00 | 0.00 H |
| ATOM | 1436 | N | PRO A | 98121.906 | -5.725 | 10.780 | 1.00 | 0.00 N |
| ATOM | 1437 | CA | PRO A | 98120.563 | -5.349 | 10.327 | 1.00 | 0.00 C |
| ATOM | 1438 | C | PRO A | 98119.501 | -5.591 | 11.395 | 1.00 | 0.00 C |
| ATOM | 1439 | О | PRO A | 98118.481 | -4.905 | 11.436 | 1.00 | 0.00 O |
| ATOM | 1440 | CB | PRO A | 98120.328 | -6.262 | 9.121 | 1.00 | 0.00 C |
| ATOM | 1441 | CG | PRO A | 98121.691 | -6.560 | 8.604 | 1.00 | 0.00 C |
| ATOM | 1442 | CD | PRO A | 98122.594 | -6.595 | 9.805 | 1.00 | 0.00 C |
| ATOM | 1443 | HA | PRO A | 98120.526 | -4.315 | 10.012 | 1.00 | 0.00 H |
| ATOM | 1444 | 1HB | PRO A | 98119.819 | -7.160 | 9.441 | 1.00 | 0.00 H |
| ATOM | 1445 | 2HB | PRO A | 98119.730 | -5.745 | 8.386 | 1.00 | 0.00 H |
| ATOM | 1446 | 1HG | PRO A | 98121.692 | -7.519 | 8.105 | 1.00 | 0.00 H |

| ATOM | 1447 | 2HG | PRO A | 98122.004 | -5.782 | 7.922 | 1.00 | 0.00 H |
|------|--------|-----|-------|------------|--------|--------|------|--------|
| ATOM | 1448 | HD | PRO A | 98122.681 | -7.602 | 10.184 | 1.00 | 0.00 H |
| ATOM | 1449 2 | 2HD | PRO A | 98123.568 | -6.199 | 9.557 | 1.00 | 0.00 H |
| ATOM | 1450 | N | SER A | 99119.751 | -6.571 | 12.257 | 1.00 | 0.00 N |
| ATOM | 1451 | CA | SER A | 99118.818 | -6.903 | 13.328 | 1.00 | 0.00 C |
| ATOM | 1452 | C | SER A | 99119.407 | -6.553 | 14.690 | 1.00 | 0.00 C |
| ATOM | 1453 | O | SER A | 99120.557 | -6.884 | 14.983 | 1.00 | 0.00 O |
| ATOM | 1454 | СВ | SER A | 99118.462 | -8.390 | 13.279 | 1.00 | 0.00 C |
| ATOM | 1455 | OG | SER A | 99118.677 | -8.924 | 11.984 | 1.00 | 0.00 O |
| ATOM | 1456 | Н | SER A | 99120.583 | -7.081 | 12.174 | 1.00 | 0.00 H |
| ATOM | 1457 | НА | SER A | 99117.920 | -6.322 | 13.178 | 1.00 | 0.00 H |
| ATOM | 1458 | lНВ | SER A | 99119.079 | -8.929 | 13.983 | 1.00 | 0.00 H |
| ATOM | 1459 2 | 2HB | SER A | 99117.422 | -8.518 | 13.540 | 1.00 | 0.00 H |
| ATOM | 1460 | HG | SER A | 99119.277 | -9.671 | 12.041 | 1.00 | 0.00 H |
| ATOM | 1461 | N | GLY A | 100118.614 | -5.885 | 15.520 | 1.00 | 0.00 N |
| ATOM | 1462 | CA | GLY A | 100119.076 | -5.501 | 16.842 | 1.00 | 0.00 C |
| ATOM | 1463 | C | GLY A | 100118.068 | -5.831 | 17.927 | 1.00 | 0.00 C |
| ATOM | 1464 | O | GLY A | 100116.862 | -5.824 | 17.680 | 1.00 | 0.00 O |
| ATOM | 1465 | Н | GLY A | 100117.707 | -5.647 | 15.233 | 1.00 | 0.00 H |
| ATOM | 1466 | IHA | GLY A | 100119.999 | -6.020 | 17.052 | 1.00 | 0.00 H |
| ATOM | 1467 2 | 2HA | GLY A | 100119.262 | -4.437 | 16.850 | 1.00 | 0.00 H |
| ATOM | 1468 | N | PRO A | 101118.536 | -6.127 | 19.153 | 1.00 | 0.00 N |
| ATOM | 1469 | CA | PRO A | 101117.654 | -6.460 | 20.276 | 1.00 | 0.00 C |
| ATOM | 1470 | C | PRO A | 101116.891 | -5.245 | 20.792 | 1.00 | 0.00 C |
| ATOM | 1471 | О | PRO A | 101117.052 | -4.840 | 21.944 | 1.00 | 0.00 O |
| ATOM | 1472 | СВ | PRO A | 101118.620 | -6.980 | 21.341 | 1.00 | 0.00 C |
| ATOM | 1473 | CG | PRO A | 101119.916 | -6.311 | 21.034 | 1.00 | 0.00 C |

| ATOM | 1474 | CD | PRO A 101119.960 | -6.160 | 19.538 | 1.00 | 0.00 C |
|------|--------|-----|------------------|--------|--------|------|--------|
| ATOM | 1475 | НА | PRO A 101116.954 | -7.238 | 20.010 | 1.00 | 0.00 H |
| ATOM | 1476 | lНВ | PRO A 101118.258 | -6.710 | 22.322 | 1.00 | 0.00 H |
| ATOM | 1477 | 2HB | PRO A 101118.705 | -8.054 | 21.263 | 1.00 | 0.00 H |
| ATOM | 1478 | lHG | PRO A 101119.950 | -5.343 | 21.511 | 1.00 | 0.00 H |
| ATOM | 1479 | 2HG | PRO A 101120.736 | -6.926 | 21.373 | 1.00 | 0.00 H |
| ATOM | 1480 | IHD | PRO A 101120.453 | -5.238 | 19.267 | 1.00 | 0.00 H |
| ATOM | 1481 2 | 2HD | PRO A 101120.461 | -7.003 | 19.088 | 1.00 | 0.00 H |
| ATOM | 1482 | N | SER A 102116.057 | -4.667 | 19.933 | 1.00 | 0.00 N |
| ATOM | 1483 | CA | SER A 102115.268 | -3.498 | 20.303 | 1.00 | 0.00 C |
| ATOM | 1484 | C | SER A 102113.913 | -3.913 | 20.867 | 1.00 | 0.00 C |
| ATOM | 1485 | O | SER A 102113.606 | -3.648 | 22.030 | 1.00 | 0.00 O |
| ATOM | 1486 | CB | SER A 102115.071 | -2.585 | 19.091 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102114.531 | -1.334 | 19.478 | 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102115.971 | -5.036 | 19.029 | 1.00 | 0.00 H |
| ATOM | 1489 | HA | SER A 102115.812 | -2.959 | 21.064 | 1.00 | 0.00 H |
| ATOM | 1490 | lНВ | SER A 102116.024 | -2.418 | 18.611 | 1.00 | 0.00 H |
| ATOM | 1491 2 | 2HB | SER A 102114.394 | -3.057 | 18.394 | 1.00 | 0.00 H |
| ATOM | 1492 | HG | SER A 102115.179 | -0.642 | 19.319 | 1.00 | 0.00 H |
| ATOM | 1493 | N | SER A 103113.105 | -4.563 | 20.036 | 1.00 | 0.00 N |
| ATOM | 1494 | CA | SER A 103111.783 | -5.015 | 20.452 | 1.00 | 0.00 C |
| ATOM | 1495 | C | SER A 103111.266 | -6.112 | 19.527 | 1.00 | 0.00 C |
| ATOM | 1496 | O | SER A 103111.769 | -6.290 | 18.418 | 1.00 | 0.00 O |
| ATOM | 1497 | CB | SER A 103110.802 | -3.840 | 20.466 | 1.00 | 0.00 C |
| ATOM | 1498 | OG | SER A 103111.343 | -2.733 | 21.164 | 1.00 | 0.00 O |
| ATOM | 1499 | Н | SER A 103113.407 | -4.745 | 19.121 | 1.00 | 0.00 H |
| ATOM | 1500 | НА | SER A 103111.868 | -5.413 | 21.452 | 1.00 | 0.00 H |

ATOM SER A 103110.587 -3.541 19.452 1.00 0.00 H 1501 1HB **ATOM** SER A 103109.887 -4.146 20.952 1.00 0.00 H1502 2HB **ATOM** HG SER A 103111.681 -3.022 22.014 1.00 0.00 H 1503 1504 N GLY A 104110.261 -6.846 19.992 1.00 0.00 N **ATOM ATOM** 1505 CA GLY A 104109.694 -7.916 19.194 1.00 0.00 C 1506 C GLY A 104108.344 -8.374 19.712 1.00 0.00 C **ATOM** 1507 O GLY A 104108.159 -9.597 19.890 1.00 0.00 O **ATOM ATOM** 1508 OXT GLY A 104107.472 -7.510 19.941 1.00 0.00 O 1509 H GLY A 104109.901 -6.658 20.885 1.00 0.00 H **ATOM** 1510 1HA GLY A 104109.578 -7.571 18.178 1.00 0.00 H**ATOM ATOM** 1511 2HA GLY A 104110.373 -8.756 19.203 1.00 0.00 H 1512 GLY A 104 TER

ENDMDL

Three-Dimensional Structure Coordinate Table 6

0.00 N ATOM 1 N GLY A 1112.318 9.750 - 2.270 1.00 1111.240 0.00 C ATOM 2 CA GLY A 9.201 -3.139 1.00 1.00 0.00 C ATOM 3 C GLY A 1110.691 7.886 -2.623 7.663 -2.635 1.00 0.00 O ATOM 4 O **GLY A** 1109.480 9.172 -2.358 1.00 0.00 H ATOM 5 1H GLY A 1113.178 ATOM 62H GLY A 1112.012 9.746 -1.276 1.00 0.00 H10.727 -2.549 1.00 0.00 H ATOM 73H GLY A 1112.539 ATOM 8 1HA GLY A 1110.435 9.918 -3.192 1.00 0.00 H 1.00 0.00 H ATOM 9 2HA GLY A 1111.637 9.047 -4.132 1.00 0.00 N 7.013 -2.167 ATOM10 N SER A 2111.584 5.712 -1.643 1.00 0.00 C ATOM11 CA SER A 2111.182 0.00 C 2112.008 5.342 -0.415 1.00 ATOM12 C SER A

| ATOM13 | О | SER A | 2111.463 | 4.944 | 0.615 | 1.00 | 0.00 O |
|--------|-----|-------|----------|-------|--------|------|--------|
| ATOM14 | СВ | SER A | 2111.337 | 4.636 | -2.718 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2110.409 | 4.831 | -3.772 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2112.534 | 7.249 | -2.182 | 1.00 | 0.00 H |
| ATOM17 | HA | SER A | 2110.143 | 5.776 | -1.357 | 1.00 | 0.00 H |
| ATOM18 | 1HB | SER A | 2112.337 | 4.677 | -3.125 | 1.00 | 0.00 H |
| ATOM19 | 2HB | SER A | 2111.166 | 3.664 | -2.280 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2109.545 | 5.031 | -3.405 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3113.325 | 5.477 | -0.531 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3114.226 | 5.157 | 0.571 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3114.354 | 6.336 | 1.530 | 1.00 | 0.00 C |
| ATOM24 | Ο | SER A | 3114.036 | 6.223 | 2.713 | 1.00 | 0.00 O |
| ATOM25 | CB | SER A | 3115.604 | 4.770 | 0.033 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3116.188 | 5.838 | -0.692 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3113.700 | 5.799 | 1.377 | 1.00 | 0.00 H |
| ATOM28 | НА | SER A | 3113.809 | 4.316 | 1.105 | 1.00 | 0.00 H |
| ATOM29 | 1HB | SER A | 3116.252 | 4.515 | 0.859 | 1.00 | 0.00 H |
| ATOM30 | 2HB | SER A | 3115.506 | 3.917 | -0.623 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3117.117 | 5.913 | -0.460 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4114.820 | 7.466 | 1.009 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4114.983 | 8.649 | 1.833 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4116.174 | 8.550 | 2.765 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4116.069 | 8.004 | 3.863 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4115.058 | 7.497 | 0.060 | 1.00 | 0.00 H |
| ATOM37 | 1HA | GLY A | 4115.113 | 9.507 | 1.190 | 1.00 | 0.00 H |
| ATOM38 | 2HA | GLY A | 4114.089 | 8.787 | 2.424 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5117.312 | 9.078 | 2.326 | 1.00 | 0.00 N |

| ATOM40 | CA | SER A | 5118.529 | 9.046 | 3.127 | 1.00 | 0.00 C |
|--------|-----|-------|----------|--------|-------|------|--------|
| ATOM41 | C | SER A | 5119.241 | 10.395 | 3.092 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5119.252 | 11.074 | 2.066 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5119.468 | 7.948 | 2.623 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5119.748 | 8.109 | 1.244 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5117.334 | 9.500 | 1.441 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5118.249 | 8.827 | 4.147 | 1.00 | 0.00 H |
| ATOM47 | 1HB | SER A | 5120.397 | 7.991 | 3.173 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5119.006 | 6.984 | 2.774 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5120.660 | 7.865 | 1.070 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6119.832 | 10.776 | 4.219 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6120.546 | 12.044 | 4.317 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6121.965 | 11.832 | 4.834 | 1.00 | 0.00 C |
| ATOM53 | О | SER A | 6122.531 | 12.701 | 5.498 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6119.794 | 13.006 | 5.238 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6118.457 | 13.187 | 4.805 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6119.789 | 10.190 | 5.003 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6120.597 | 12.473 | 3.327 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6119.782 | 12.606 | 6.240 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6120.292 | 13.964 | 5.238 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6118.443 | 13.319 | 3.854 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7122.535 | 10.671 | 4.527 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7123.883 | 10.367 | 4.969 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7124.017 | 8.950 | 5.488 | 1.00 | 0.00 C |
| ATOM64 | O | GLY A | 7123.400 | 8.587 | 6.490 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7122.036 | 10.016 | 3.995 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7124.561 | 10.500 | 4.139 | 1.00 | 0.00 H |

| ATOM67 | 2HA | GLY A | 7124.155 | 11.054 | 5.756 | 1.00 | 0.00 H |
|--------|------|-------|----------|--------|-------|------|--------|
| ATOM68 | N | LEU A | 8124.825 | 8.144 | 4.805 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8125.038 | 6.758 | 5.203 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8126.306 | 6.621 | 6.038 | 1.00 | 0.00 C |
| ATOM71 | O | LEU A | 8126.247 | 6.510 | 7.263 | 1.00 | 0.00 O |
| ATOM72 | СВ | LEU A | 8125.123 | 5.858 | 3.969 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8123.782 | 5.319 | 3.467 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8123.953 | 4.629 | 2.123 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8123.178 | 4.364 | 4.486 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8125.289 | 8.492 | 4.014 | 1.00 | 0.00 H |
| ATOM77 | HA | LEU A | 8124.196 | 6.453 | 5.801 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8125.583 | 6.421 | 3.169 | 1.00 | 0.00 H |
| ATOM79 | 2HB | LEU A | 8125.757 | 5.017 | 4.205 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8123.097 | 6.144 | 3.333 | 1.00 | 0.00 H |
| ATOM81 | 1HD1 | LEU A | 8123.170 | 3.896 | 1.992 | 1.00 | 0.00 H |
| ATOM82 | 2HD1 | LEU A | 8124.915 | 4.140 | 2.089 | 1.00 | 0.00 H |
| ATOM83 | 3HD1 | LEU A | 8123.893 | 5.362 | 1.331 | 1.00 | 0.00 H |
| ATOM84 | 1HD2 | LEU A | 8123.006 | 4.890 | 5.414 | 1.00 | 0.00 H |
| ATOM85 | 2HD2 | LEU A | 8123.859 | 3.544 | 4.658 | 1.00 | 0.00 H |
| ATOM86 | 3HD2 | LEU A | 8122.241 | 3.982 | 4.110 | 1.00 | 0.00 H |
| ATOM87 | N | ALA A | 9127.450 | 6.628 | 5.367 | 1.00 | 0.00 N |
| ATOM88 | CA | ALAA | 9128.735 | 6.505 | 6.044 | 1.00 | 0.00 C |
| ATOM89 | C | ALA A | 9129.891 | 6.773 | 5.085 | 1.00 | 0.00 C |
| ATOM90 | Ο | ALA A | 9130.601 | 5.854 | 4.679 | 1.00 | 0.00 O |
| ATOM91 | CB | ALA A | 9128.872 | 5.123 | 6.665 | 1.00 | 0.00 C |
| ATOM92 | Н | ALA A | 9127.429 | 6.720 | 4.392 | 1.00 | 0.00 H |
| ATOM93 | НА | ALA A | 9128.764 | 7.235 | 6.839 | 1.00 | 0.00 H |

| ATOM94 1 | HB | ALA | Α | 912 | 7.891 | 4.72 | 4 (| 6.876 | 1.00 | 0.00 | Н |
|----------|------|-----|----|-------|--------|-------|-------|--------------|-------|------|--------|
| ATOM95 2 | HB | ALA | Α | 9129 | 9.436 | 5.19 | 5 | 7.583 | 1.00 | 0.00 | Н |
| ATOM96 3 | НВ | ALA | Α | 9129 | 9.387 | 4.46 | 8 : | 5.978 | 1.00 | 0.00 | Н |
| ATOM97 | N | MET | Ά | 1013 | 0.074 | 8.04 | 1 | 4.727 | 1.00 | 0.00 | N |
| ATOM98 | CA | MET | `A | 1013 | 1.144 | 8.42 | 29 | 3.816 | 1.00 | 0.00 | C |
| ATOM99 | C | MET | Α | 1013 | 1.191 | 9.94 | 6 | 3.646 | 1.00 | 0.00 | C |
| ATOM | 100 | O | MI | ET A | 10130 | .954 | 10.4 | 65 | 2.554 | 1.00 | 0.00 O |
| ATOM | 101 | СВ | M | ET A | 10130 |).955 | 7.7 | ' 54 | 2.457 | 1.00 | 0.00 C |
| ATOM | 102 | CG | M | ET A | 10129 | 9.539 | 7.8 | 363 | 1.913 | 1.00 | 0.00 C |
| ATOM | 103 | SD | MI | ET A | 10129 | .407 | 9.0 | 23 | 0.539 | 1.00 | 0.00 S |
| ATOM | 104 | CE | MI | ET A | 10129 | 0.163 | 7.8 | 97 - | 0.833 | 1.00 | 0.00 C |
| ATOM | 105 | Н | MI | ET A | 10129 | .476 | 8.7 | 29 | 5.084 | 1.00 | 0.00 H |
| ATOM | 106 | НА | M | ET A | 10132 | 2.078 | 8.0 |)99 | 4.245 | 1.00 | 0.00 H |
| ATOM | 107 | 1HB | ME | ET A | 10131 | .628 | 8.2 | 10 | 1.746 | 1.00 | 0.00 H |
| ATOM | 108 | 2HB | ME | ET A | 10131 | .202 | 6.7 | 07 | 2.551 | 1.00 | 0.00 H |
| ATOM | 109 | 1HG | MI | ET A | 10129 | .223 | 6.8 | 88 | 1.573 | 1.00 | 0.00 H |
| ATOM | 110 | 2HG | ME | ET A | 10128 | .887 | 8.1 | 93 | 2.709 | 1.00 | 0.00 H |
| ATOM | 111 | 1HE | ME | TA | 10130 | .124 | 7.58 | 37 -1 | 1.218 | 1.00 | 0.00 H |
| ATOM | 112 | 2HE | ME | ETA | 10128 | .607 | 8.39 | 95 - | 1.613 | 1.00 | 0.00 H |
| ATOM | 113 | 3HE | ME | ET A | 10128 | .615 | 7.03 | 31 -(| 0.494 | 1.00 | 0.00 H |
| ATOM | .114 | N | PR | OA | 11131. | .502 | 10.68 | 32 | 4.727 | 1.00 | 0.00 N |
| ATOM | 115 | CA | PR | A O. | 11131 | .579 | 12.1 | 45 | 4.688 | 1.00 | 0.00 C |
| ATOM | 116 | C | PR | ΟA | 11132. | 593 | 12.64 | 15 | 3.660 | 1.00 | 0.00 C |
| ATOM | 11,7 | О | PR | OA | 11132. | .293 | 13.54 | 14 | 2.875 | 1.00 | 0.00 O |
| ATOM | 118 | CB | PR | A O.A | 11132 | .019 | 12.5 | 34 | 6.104 | 1.00 | 0.00 C |
| ATOM | 119 | CG | PR | RO A | 11131 | .698 | 11.3 | 52 | 6.955 | 1.00 | 0.00 C |
| ATOM | 120 | CD | PF | ROA | 11131 | .801 | 10.1 | 45 | 6.065 | 1.00 | 0.00 C |

| ATOM | 121 HA | PRO A | 11130.615 | 12.582 | 4.476 | 1.00 | 0.00 H |
|------|---------|-------|-----------|--------|--------|------|--------|
| ATOM | 122 1HB | PRO A | 11133.076 | 12.749 | 6.109 | 1.00 | 0.00 H |
| ATOM | 123 2HB | PRO A | 11131.469 | 13.407 | 6.424 | 1.00 | 0.00 H |
| ATOM | 124 1HG | PRO A | 11132.411 | 11.280 | 7.761 | 1.00 | 0.00 H |
| ATOM | 125 2HG | PRO A | 11130.696 | 11.444 | 7.348 | 1.00 | 0.00 H |
| ATOM | 126 1HD | PRO A | 11132.798 | 9.733 | 6.102 | 1.00 | 0.00 H |
| ATOM | 127 2HD | PRO A | 11131.072 | 9.402 | 6.353 | 1.00 | 0.00 H |
| ATOM | 128 N | PRO A | 12133.809 | 12.066 | 3.642 | 1.00 | 0.00 N |
| ATOM | 129 CA | PRO A | 12134.853 | 12.465 | 2.692 | 1.00 | 0.00 C |
| ATOM | 130 C | PRO A | 12134.377 | 12.375 | 1.247 | 1.00 | 0.00 C |
| ATOM | 131 O | PRO A | 12134.926 | 13.028 | 0.359 | 1.00 | 0.00 O |
| ATOM | 132 CB | PRO A | 12135.981 | 11.461 | 2.945 | 1.00 | 0.00 C |
| ATOM | 133 CG | PRO A | 12135.751 | 10.969 | 4.331 | 1.00 | 0.00 C |
| ATOM | 134 CD | PRO A | 12134.262 | 10.980 | 4.532 | 1.00 | 0.00 C |
| ATOM | 135 HA | PRO A | 12135.206 | 13.467 | 2.892 | 1.00 | 0.00 H |
| ATOM | 136 1HB | PRO A | 12135.918 | 10.658 | 2.225 | 1.00 | 0.00 H |
| ATOM | 137 2HB | PRO A | 12136.935 | 11.957 | 2.856 | 1.00 | 0.00 H |
| ATOM | 138 1HG | PRO A | 12136.135 | 9.965 | 4.434 | 1.00 | 0.00 H |
| ATOM | 139 2HG | PRO A | 12136.229 | 11.629 | 5.040 | 1.00 | 0.00 H |
| ATOM | 140 1HD | PRO A | 12133.834 | 10.034 | 4.236 | 1.00 | 0.00 H |
| ATOM | 141 2HD | PRO A | 12134.023 | 11.198 | 5.561 | 1.00 | 0.00 H |
| ATOM | 142 N | GLY A | 13133.351 | 11.559 | 1.017 | 1.00 | 0.00 N |
| ATOM | 143 CA | GLY A | 13132.818 | 11.397 | -0.322 | 1.00 | 0.00 C |
| ATOM | 144 C | GLY A | 13133.068 | 10.012 | -0.886 | 1.00 | 0.00 C |
| ATOM | 145 O | GLY A | 13132.330 | 9.545 | -1.754 | 1.00 | 0.00 O |
| ATOM | 146 H | GLY A | 13132.954 | 11.064 | 1.765 | 1.00 | 0.00 H |
| ATOM | 147 1HA | GLY A | 13131.753 | 11.577 | -0.298 | 1.00 | 0.00 H |
| | | | | | | | |

| ATOM | 148 | 2HA | GLY A | 13133.278 | 12.127 | -0.972 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 149 | N | ASNA | 14134.112 | 9.353 | -0.393 | 1.00 | 0.00 N |
| ATOM | 150 | | ASNA | 14134.459 | 8.014 | -0.854 | 1.00 | 0.00 C |
| | | | | | | | | |
| ATOM | 151 | С | ASN A | 14133.299 | 7.045 | -0.640 | 1.00 | 0.00 C |
| ATOM | 152 | О | ASN A | 14132.195 | 7.453 | -0.284 | 1.00 | 0.00 O |
| ATOM | 153 | CB | ASN A | 14135.703 | 7.506 | -0.122 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14136.823 | 8.529 | -0.108 | 1.00 | 0.00 C |
| ATOM | 155 | OD1 | ASN A | 14136.609 | 9.697 | 0.216 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14138.026 | 8.093 | -0.460 | 1.00 | 0.00 N |
| ATOM | 157 | Н | ASN A | 14134.664 | 9.778 | 0.297 | 1.00 | 0.00 H |
| ATOM | 158 | НА | ASN A | 14134.672 | 8.072 | -1.911 | 1.00 | 0.00 H |
| ATOM | 159 | 1HB | ASN A | 14135.442 | 7.272 | 0.899 | 1.00 | 0.00 H |
| ATOM | 160 | 2HB | ASN A | 14136.062 | 6.613 | -0.612 | 1.00 | 0.00 H |
| ATOM | 161 | 1HD2 | ASN A | 14138.123 | 7.149 | -0.706 | 1.00 | 0.00 H |
| ATOM | 162 | 2HD2 | ASN A | 14138.769 | 8.733 | -0.460 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15133.559 | 5.761 | -0.861 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15132.538 | 4.734 | -0.693 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15132.234 | 4.506 | 0.785 | 1.00 | 0.00 C |
| ATOM | 166 | O | SER A | 15131.163 | 4.867 | 1.271 | 1.00 | 0.00 O |
| ATOM | 167 | СВ | SER A | 15132.989 | 3.423 | -1.341 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15132.025 | 2.403 | -1.154 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15134.460 | 5.496 | -1.144 | 1.00 | 0.00 H |
| ATOM | 170 | НА | SER A | 15131.639 | 5.077 | -1.184 | 1.00 | 0.00 H |
| ATOM | 171 | 1HB | SER A | 15133.130 | 3.578 | -2.400 | 1.00 | 0.00 H |
| ATOM | 172 | 2HB | SER A | 15133.921 | 3.108 | -0.896 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15132.121 | 2.027 | -0.276 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16133.184 | 3.902 | 1.492 | 1.00 | 0.00 N |

| ATOM | 175 | CA | HIS A | 16133.019 | 3.626 | 2.914 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|-------|------|--------|
| ATOM | 176 | C | HIS A | 16133.864 | 4.578 | 3.754 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.441 | 5.026 | 4.820 | 1.00 | 0.00 O |
| ATOM | 178 | СВ | HIS A | 16133.401 | 2.176 | 3.221 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16132.222 | 1.262 | 3.354 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16131.448 | 1.193 | 4.493 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16131.686 | 0.375 | 2.482 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16130.487 | 0.303 | 4.316 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16130.610 | -0.207 | 3.104 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16134.016 | 3.638 | 1.047 | 1.00 | 0.00 H |
| ATOM | 185 | НА | HIS A | 16131.978 | 3.775 | 3.162 | 1.00 | 0.00 H |
| ATOM | 186 1 | HB | HIS A | 16134.024 | 1.800 | 2.424 | 1.00 | 0.00 H |
| ATOM | 187 2 | HB | HIS A | 16133.953 | 2.144 | 4.149 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16131.582 | 1.718 | 5.309 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16132.040 | 0.165 | 1.482 | 1.00 | 0.00 H |
| ATOM | 190 | HE1 | HIS A | 16129.730 | 0.038 | 5.039 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16129.981 | -0.833 | 2.688 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.063 | 4.882 | 3.267 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17135.949 | 5.778 | 3.985 | 1.00 | 0.00 C |
| ATOM | 194 | C | GLY A | 17137.401 | 5.349 | 3.901 | 1.00 | 0.00 C |
| ATOM | 195 | О | GLY A | 17138.064 | 5.173 | 4.923 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.348 | 4.495 | 2.413 | 1.00 | 0.00 H |
| ATOM | 197 1 | HA | GLY A | 17135.854 | 6.771 | 3.570 | 1.00 | 0.00 H |
| ATOM | 198 2 | HA | GLY A | 17135.654 | 5.805 | 5.024 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18137.897 | 5.182 | 2.678 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.279 | 4.771 | 2.465 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.246 | 5.872 | 2.888 | 1.00 | 0.00 C |

| ATOM | 202 | O | LEU A | 18140.497 | 6.814 | 2.136 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|-------|---------|------|--------|
| ATOM | 203 | CB | LEU A | 18139.506 | 4.415 | 0.994 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18138.484 | 3.445 | 0.398 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18138.481 | 3.540 | -1.120 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18138.781 | 2.021 | 0.844 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.318 | 5.338 | 1.903 | 1.00 | 0.00 H |
| ATOM | 208 | HA | LEU A | 18139.462 | 3.895 | 3.070 | 1.00 | 0.00 H |
| ATOM | 209 | 1HB | LEU A | 18139.484 | 5.328 | 0.417 | 1.00 | 0.00 H |
| ATOM | 210 | 2HB | LEU A | 18140.486 | 3.972 | 0.900 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18137.498 | 3.709 | 0.751 | 1.00 | 0.00 H |
| ATOM | 212 | 1HD1 | LEU A | 18138.860 | 4.506 | -1.421 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18137.472 | 3.419 | -1.485 | 1.00 | 0.00 H |
| ATOM | 214 | 3HD1 | LEU A | 18139.109 | 2.763 | - 1.530 | 1.00 | 0.00 H |
| ATOM | 215 | 1HD2 | LEU A | 18139.591 | 1.619 | 0.254 | 1.00 | 0.00 H |
| ATOM | 216 | 2HD2 | LEU A | 18137.899 | 1.411 | 0.709 | 1.00 | 0.00 H |
| ATOM | 217 | 3HD2 | LEU A | 18139.061 | 2.021 | 1.887 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19140.783 | 5.748 | 4.096 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.722 | 6.733 | 4.621 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19142.809 | 6.061 | 5.452 | 1.00 | 0.00 C |
| ATOM | 221 | Ο | GLU A | 19142.810 | 4.843 | 5.622 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19140.984 | 7.772 | 5.467 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.233 | 7.174 | 6.645 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19139.754 | 8.226 | 7.625 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19140.533 | 9.155 | 7.928 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19138.599 | 8.123 | 8.091 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.544 | 4.976 | 4.650 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.184 | 7.230 | 3.779 | 1,00 | 0.00 H |

| ATOM | 229 | 1HB | GLU A | 19141.702 | 8.483 | 5.849 | 1.00 | 0.00 H |
|------|-----|------|--------|-----------|-------|--------|------|--------|
| ATOM | 230 | 2HB | GLU A | 19140.274 | 8.291 | 4.841 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.375 | 6.635 | 6.272 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19140.888 | 6.490 | 7.164 | 1.00 | 0.00 H |
| ATOM | 233 | N | VALA | 20143.732 | 6.865 | 5.969 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VALA | 20144.825 | 6.349 | 6.785 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.297 | 5.620 | 8.015 | 1.00 | 0.00 C |
| ATOM | 236 | O | VALA | 20143.530 | 6.181 | 8.799 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20145.770 | 7.479 | 7.235 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VALA | 20146.993 | 6.908 | 7.939 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VALA | 20146.181 | 8.337 | 6.049 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.678 | 7.829 | 5.798 | 1.00 | 0.00 H |
| ATOM | 241 | HA | VAL A | 20145.391 | 5.654 | 6.182 | 1.00 | 0.00 H |
| ATOM | 242 | HB | .VAL A | 20145.240 | 8.105 | 7.938 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20146.795 | 6.830 | 8.997 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20147.838 | 7.559 | 7.777 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20147.211 | 5.928 | 7.540 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20145.398 | 9.046 | 5.828 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20146.348 | 7.705 | 5.189 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20147.091 | 8.868 | 6.287 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.711 | 4.369 | 8.179 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.269 | 3.583 | 9.316 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.228 | 2.548 | 8.939 | 1.00 | 0.00 C |
| ATOM | 252 | Ο | GLY A | 21143.210 | 1.447 | 9.489 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.322 | 3.975 | 7.522 | 1.00 | 0.00 H |
| ATOM | 254 | 1HA | GLY A | 21145.123 | 3.080 | 9.745 | 1.00 | 0.00 H |
| ATOM | 255 | 2HA | GLY A | 21143.847 | 4.248 | 10.056 | 1.00 | 0.00 H |

| ATOM | 256 | N | SER A | 22142.359 | 2.901 | 7.997 | 1.00 | 0.00 N |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 257 | CA | SER A | 22141.310 | 1.995 | 7.546 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.877 | 0.922 | 6.622 | 1.00 | 0.00 C |
| ATOM | 259 | О | SER A | 22142.764 | 1.192 | 5.812 | 1.00 | 0.00 O |
| ATOM | 260 | CB | SER A | 22140.208 | 2.774 | 6.826 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22139.268 | 3.299 | 7.747 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.425 | 3.793 | 7.596 | 1.00 | 0.00 H |
| ATOM | 263 | HA | SER A | 22140.889 | 1.516 | 8.417 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.649 | 3.592 | 6.276 | 1.00 | 0.00 H |
| ATOM | 265 | 2HB | SER A | 22139.694 | 2.116 | 6.141 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22138.475 | 3.569 | 7.277 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.359 | -0.295 | 6.749 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.815 | -1.410 | 5.924 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.296 | -1.278 | 4.496 | 1.00 | 0.00 C |
| ATOM | 270 | О | LEU A | 23140.234 | -0.702 | 4.261 | 1.00 | 0.00 O |
| AŤOM | 271 | СВ | LEU A | 23141.353 | -2.738 | 6.526 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23141.931 | -3.059 | 7.905 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23140.954 | -3.903 | 8.709 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23143.268 | -3.773 | 7.769 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.655 | -0.449 | 7.412 | 1.00 | 0.00 H |
| ATOM | 276 | HA | LEU A | 23142.894 | -1.388 | 5.907 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.276 | -2.718 | 6.605 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.633 | -3.531 | 5.850 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.096 | -2.137 | 8.443 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23140.921 | -4.902 | 8.302 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23139.970 | -3.460 | 8.659 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23141.277 | -3.944 | 9.739 | 1.00 | 0.00 H |

| ATOM | 283 | 1HD2 | LEU A | 23143.908 | -3.500 | 8.594 | 1.00 | 0.00 H |
|--------|-----|------------|-------|-----------|--------|--------|------|--------|
| ATOM | 284 | 2HD2 | LEU A | 23143.736 | -3.485 | 6.840 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23143.107 | -4.841 | 7.776 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.055 | -1.814 | 3.546 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.672 | -1.757 | 2.140 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.245 | -2.941 | 1.367 | 1.00 | 0.00 C |
| ATOM | 289 | O . | ALA A | 24143.206 | -3.573 | 1.804 | 1.00 | 0.00 O |
| ATOM | 290 | CB | ALA A | 24142.135 | -0.447 | 1.520 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.890 | -2.260 | 3.795 | 1.00 | 0.00 H |
| ATOM | 292 | HA | ALA A | 24140.593 | -1.793 | 2.086 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALA A | 24143.026 | -0.105 | 2.025 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24141.356 | 0.295 | 1.623 | 1.00 | 0.00 H |
| ATOM | 295 | 3НВ | ALA A | 24142.350 | -0.601 | 0.473 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.647 | -3.236 | 0.217 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.098 | -4.344 | -0.617 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.441 | -3.863 | -2.023 | 1.00 | 0.00 C |
| ATOM | 299 | Ο | GLU A | 25141.810 | -2.945 | -2.547 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25141.023 | -5.430 | -0.684 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.523 | -6.747 | -1.252 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.399 | -7.623 | -1.770 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25140.407 | -7.947 | -2.976 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25139.511 | -7.986 | -0.970 | 1.00 | 0.00 O |
| ATOM | 305 | Н | GLU A | 25140.885 | -2.695 | -0.079 | 1.00 | 0.00 H |
| ATOM | 306 | HA | GLU A | 25142.987 | -4.758 | -0.164 | 1.00 | 0.00 H |
| ATOM | 307 | 1HB | GLU A | 25140.646 | -5.611 | 0.311 | 1.00 | 0.00 H |
| ATOM · | 308 | 2HB | GLU A | 25140.212 | -5.078 | -1.306 | 1.00 | 0.00 H |
| ATOM | 309 | 1HG | GLU A | 25142.200 | -6.540 | -2.066 | 1.00 | 0.00 H |

| ATOM | 310 | 2HG | GLU A | 25142.048 | -7.283 | -0.475 | 1.00 | 0.00 H |
|------|-----|------|---------|-----------|--------|--------|------|--------|
| ATOM | 311 | N | VAL A | 26143.445 | -4.489 | -2.629 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.872 | -4.124 | -3.974 | 1.00 | 0.00 C |
| ATOM | 313 | C | VALA | 26143.444 | -5.178 | -4.990 | 1.00 | 0.00 C |
| ATOM | 314 | Ο | VAL A | 26143.415 | -6.370 | -4.688 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VAL A | 26145.399 | -3.944 | -4.051 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VALA | 26145.804 | -3.375 | -5.401 | 1.00 | 0.00 C |
| ATOM | 317 | CG2 | 2 VAL A | 26145.890 | -3.054 | -2.919 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.910 | -5.212 | -2.160 | 1.00 | 0.00 H |
| ATOM | 319 | HA | VAL A | 26143.406 | -3.183 | -4.229 | 1.00 | 0.00 H |
| ATOM | 320 | HB | VAL A | 26145.861 | -4.915 | -3.942 | 1.00 | 0.00 H |
| ATOM | 321 | 1HG1 | VAL A | 26146.882 | -3.336 | -5.467 | 1.00 | 0.00 H |
| ATOM | 322 | 2HG1 | VAL A | 26145.401 | -2.378 | -5.506 | 1.00 | 0.00 H |
| ATOM | 323 | 3HG1 | VAL A | 26145.418 | -4.005 | -6.188 | 1.00 | 0.00 H |
| ATOM | 324 | 1HG2 | VAL A | 26145.976 | -3.637 | -2.013 | 1.00 | 0.00 H |
| ATOM | 325 | 2HG2 | VAL A | 26145.186 | -2.250 | -2.763 | 1.00 | 0.00 H |
| ATOM | 326 | 3HG2 | VAL A | 26146.855 | -2.643 | -3.175 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYS A | 27143.116 | -4.729 | -6.197 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27142.690 | -5.633 | -7.259 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27143.880 | -6.082 | -8.101 | 1.00 | 0.00 C |
| ATOM | 330 | O | LYS A | 27144.102 | -5.577 | -9.201 | 1.00 | 0.00 O |
| ATOM | 331 | CB | LYS A | 27141.647 | -4.954 | -8.149 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.301 | -4.761 | -7.470 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27139.285 | -5.786 | -7.945 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27139.368 | -7.071 | -7.135 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27138.350 | -7.109 | -6.048 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27143.160 | -3.766 | -6.378 | 1.00 | 0.00 H |

| ATOM | 337 | HA | LYSA | 27142.245 | -6.501 | -6.796 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|---------|------|--------|
| ATOM | 338 | 1HB | LYS A | 27142.021 | -3.983 | -8.443 | 1.00 | 0.00 H |
| ATOM | 339 2 | 2HB | LYS A | 27141.499 | -5.556 | -9.034 | 1.00 | 0.00 H |
| ATOM | 340 | IHG | LYSA | 27140.429 | -4.864 | -6.403 | 1.00 | 0.00 H |
| ATOM | 341 2 | 2HG | LYS A | 27139.933 | -3.771 | -7.698 | 1.00 | 0.00 H |
| ATOM | 342 | IHD | LYS A | 27138.293 | -5.372 | - 7.841 | 1.00 | 0.00 H |
| ATOM | 343 2 | 2HD | LYS A | 27139.475 | -6.014 | -8.984 | 1.00 | 0.00 H |
| ATOM | 344 | 1HE | LYS A | 27139.208 | -7.909 | -7.795 | 1.00 | 0.00 H |
| ATOM | 345 2 | 2HE | LYS A | 27140.353 | -7.141 | -6.697 | 1.00 | 0.00 H |
| ATOM | 346 | ΙHZ | LYS A | 27137.554 | - 6.482 | -6.282 | 1.00 | 0.00 H |
| ATOM | 347 2 | 2HZ | LYS A | 27138.772 | -6.795 | -5.152 | 1.00 | 0.00 H |
| ATOM | 348 3 | BHZ | LYS A | 27137.992 | -8.078 | -5.928 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28144.644 | -7.034 | -7.575 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28145.812 | -7.553 | -8.278 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.714 | -9.064 | -8.456 | 1.00 | 0.00 C |
| ATOM | 352 | O | GLU A | 28144.671 | -9.664 | -8.195 | 1.00 | 0.00 O |
| ATOM | 353 | CB | GLU A | 28147.091 | -7.198 | -7.514 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28148.178 | -6.601 | -8.394 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28149.554 | -7.148 | -8.072 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28150.418 | -7.154 | -8.976 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28149.770 | -7.572 | -6.918 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.417 | -7.397 | -6.694 | 1.00 | 0.00 H |
| ATOM | 359 | НА | GLU A | 28145.846 | -7.088 | -9.252 | 1.00 | 0.00 H |
| ATOM | 360 | lНВ | GLU A | 28146.849 | -6.482 | -6.743 | 1.00 | 0.00 H |
| ATOM | 361 2 | 2HB | GLU A | 28147.483 | -8.092 | -7.052 | 1.00 | 0.00 H |
| ATOM | 362 | HG | GLU A | 28147.952 | -6.824 | -9.426 | 1.00 | 0.00 H |
| ATOM | 363 2 | 2HG | GLU A | 28148.190 | -5.530 | -8.252 | 1.00 | 0.00 H |

| ATOM | 364 | N | ASN A | 29146.807 | -9.675 | -8.902 | 1.00 | 0.00 N |
|------|-----|--------|-------|-------------|-----------|---------|------|--------|
| ATOM | 365 | CA | ASN A | 29146.843 | -11.117 | -9.113 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29146.916 | -11.858 | -7.781 | 1.00 | 0.00 C |
| ATOM | 367 | О | ASN A | 29146.049 | -12.673 | -7.467 | 1.00 | 0.00 O |
| ATOM | 368 | СВ | ASN A | 29148.038 | -11.495 | -9.992 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29147.648 | -11.689 | -11.445 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29147.487 | -12.817 - | 11.911 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29147.495 | -10.586 - | 12.168 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29147.608 | -9.143 | -9.092 | 1.00 | 0.00 H |
| ATOM | 373 | НА | ASN A | 29145.932 | -11.400 | -9.619 | 1.00 | 0.00 H |
| ATOM | 374 | 1HB | ASN A | 29148.778 | -10.711 | -9.939 | 1.00 | 0.00 H |
| ATOM | 375 | 2HB | ASN A | 29148.468 | -12.416 | -9.627 | 1.00 | 0.00 H |
| ATOM | 376 | 1HD2 / | ASN A | 29147.640 | -9.721 - | 11.730 | 1.00 | 0.00 H |
| ATOM | 377 | 2HD2 | ASN A | 29147.244 - | -10.682 - | 13.110 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30147.958 | -11.585 | -6.976 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30148.142 | -12.228 | -5.674 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30147.254 | -11.613 | -4.593 | 1.00 | 0.00 C |
| ATOM | 381 | Ο | PRO A | 30147.455 | -10.466 | -4.194 | 1.00 | 0.00 O |
| ATOM | 382 | CB | PRO A | 30149.614 | -11.962 | -5.367 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30149.906 | -10.665 | -6.040 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30149.040 | -10.624 | -7.274 | 1.00 | 0.00 C |
| ATOM | 385 | HA | PRO A | 30147.968 | -13.291 | -5.727 | 1.00 | 0.00 H |
| ATOM | 386 | 1HB | PRO A | 30149.757 | -11.895 | -4.298 | 1.00 | 0.00 H |
| ATOM | 387 | 2HB | PRO A | 30150.220 | -12.760 | -5.769 | 1.00 | 0.00 H |
| ATOM | 388 | 1HG | PRO A | 30149.657 | -9.846 | -5.381 | 1.00 | 0.00 H |
| ATOM | 389 | 2HG | PRO A | 30150.949 | -10.622 | -6.315 | 1.00 | 0.00 H |
| ATOM | 390 | 1HD | PRO A | 30148.643 | -9.631 | -7.420 | 1.00 | 0.00 H |

| ATOM | 391 2 | 2HD | PRO A | 30149.604 | -10.936 | -8.140 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|---------|------|--------|
| ATOM | 392 | N | PRO A | 31146.253 | -12.366 | -4.102 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31145.337 | -11.880 | -3.063 | 1.00 | 0.00 C |
| ATOM | 394 | C | PRO A | 31146.064 | -11.536 | -1.768 | 1.00 | 0.00 C |
| ATOM | 395 | O | PRO A | 31146.500 | -12.422 | -1.034 | 1.00 | 0.00 O |
| ATOM | 396 | СВ | PRO A | 31144.378 | -13.056 | -2.838 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31144.514 | -13.909 | -4.053 | 1.00 | 0.00 C |
| ATOM | 398 | CD | PRO A | 31145.932 | -13.743 | -4.514 | 1.00 | 0.00 C |
| ATOM | 399 | НА | PRO A | 31144.781 | -11.018 | -3.401 | 1.00 | 0.00 H |
| ATOM | 400 | НВ | PRO A | 31144.666 | -13.593 | -1.946 | 1.00 | 0.00 H |
| ATOM | 401 2 | 2HB | PRO A | 31143.369 | -12.685 | -2.730 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31144.319 | -14.940 | -3.802 | 1.00 | 0.00 H |
| ATOM | 403 2 | 2HG | PRO A | 31143.829 | -13.571 | -4.817 | 1.00 | 0.00 H |
| ATOM | 404 1 | HD | PRO A | 31146.576 | -14.455 | -4.020 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31145.997 | -13.849 | -5.586 | 1.00 | 0.00 H |
| ATOM | 406 | N | PHE A | 32146.191 | -10.242 | -1.492 | 1.00 | 0.00 N |
| ATOM | 407 | CA | PHE A | 32146.864 | -9.781 | -0.283 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32146.068 | -8.670 | 0.395 | 1.00 | 0.00 C |
| ATOM | 409 | O | PHE A | 32145.464 | -7.831 | -0.273 | 1.00 | 0.00 O |
| ATOM | 410 | СВ | PHE A | 32148.273 | -9.285 | -0.615 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.295 | -8.133 | -1.580 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32147.870 | -6.875 | -1\.187 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32148.741 | -8.311 | -2.879 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32147.889 | -5.815 | -2.073 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32148.763 | -7.254 | -3.769 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.337 | -6.004 | -3.366 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.822 | -9.581 | -2.115 | 1.00 | 0.00 H |

| ATOM | 418. | НА | PHE A | 32146.938 | -10.618 | 0.394 | 1.00 | 0.00 H |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 419 1 | НВ | PHE A | 32148.757 | -8.964 | 0.295 | 1.00 | 0.00 H |
| ATOM | 420 2 | НВ | PHE A | 32148.839 - | -10.095 | -1.050 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32147.520 | -6.724 | -0.176 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32149.076 | -9.288 | -3.196 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32147.554 | -4.838 | -1.755 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32149.113 | -7.405 | -4.780 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.352 | -5.177 | -4.059 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.071 | -8.673 | 1.724 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.349 | -7.666 | 2.492 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.315 | -6.689 | 3.153 | 1.00 | 0.00 C |
| ATOM | 429 | O . | TYR A | 33147.406 | -7.072 | 3.575 | 1.00 | 0.00 O |
| ATOM | 430 | CB | TYR A | 33144.475 | -8.335 | 3.555 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.212 | -8.953 | 2.999 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.857 | -10.258 | 3.318 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.375 | -8.232 | 2.157 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.704 | 10.828 | 2.811 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.220 | -8.794 | 1.647 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.888 | -10.091 | 1.977 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.740 | -10.655 | 1.473 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.571 | -9.369 | 2.199 | 1.00 | 0.00 H |
| ATOM | 439 | HA | TYR A | 33144.715 | -7.121 | 1.809 | 1.00 | 0.00 H |
| ATOM | 440 1 | HB | TYR A | 33145.042 | -9.116 | 4.037 | 1.00 | 0.00 H |
| ATOM | 441 2 | НВ | TYR A | 33144.188 | -7.598 | 4.290 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33143.497 | -10.832 | 3.971 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.637 | -7.216 | 1.900 | 1.00 | 0.00 H |
| ATOM | 444 | HEI | TYR A | 33141.445 | -11.844 | 3.070 | 1.00 | 0.00 H |

| ATOM | 445 | HE2 | TYR A | 33140.581 | -8.217 | 0.994 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|---------|-------|------|--------|
| ATOM | 446 | НН | TYR A | 33139.799 | -10.701 | 0.515 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.909 | -5.427 | 3.237 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.751 | -4.416 | 3.848 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34145.959 | -3.219 | 4.337 | 1.00 | 0.00 C |
| ATOM | 450 | О | GLY A | 34144.841 | -2.978 | 3.884 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.029 | -5.181 | 2.883 | 1.00 | 0.00 H |
| ATOM | 452 | 1HA | GLY A | 34147.273 | -4.856 | 4.684 | 1.00 | 0.00 H |
| ATOM | 453 | 2HA | GLY A | 34147.476 | -4.081 | 3.121 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.541 | -2.468 | 5.266 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VALA | 35145.884 | -1.291 | 5.818 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.524 | -0.008 | 5.294 | 1.00 | 0.00 C |
| ATOM | 457 | О | VAL A | 35147.743 | 0.072 | 5.144 | 1.00 | 0.00 O |
| ATOM | 458 | CB | VALA | 35145.936 | -1.289 | 7.360 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.377 | -1.253 | 7.849 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35145.140 | -0.120 | 7.925 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.434 | -2.712 | 5.588 | 1.00 | 0.00 H |
| ATOM | 462 | HA | VAL A | 35144.848 | -1.314 | 5.514 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.486 | -2.206 | 7.713 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VALA | 35147.393 | -1.031 | 8.905 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VALA | 35147.920 | -0.489 | 7.312 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VALA | 35147.841 | -2.213 | 7.675 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VALA | 35144.771 | 0.491 | 7.115 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VALA | 35145.777 | 0.476 | 8.563 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VAL A | 35144.307 | -0.497 | 8.500 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.694 | 0.991 | 5.016 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.181 | 2.269 | 4.508 | 1.00 | 0.00 C |

| ATOM | 472 | C | ILE A | 36147.115 | 2.937 | 5.513 | 1.00 | 0.00 C |
|------|-----|---------------------------|-------|-----------|-------|--------|--------|--------|
| ATOM | 473 | O | ILE A | 36146.824 | 2.986 | 6.708 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.017 | 3.229 | 4.186 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36143.994 | 2.541 | 3.278 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILE A | 36145.541 | 4.501 | 3.533 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.827 | 3.428 | 2.903 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.733 | 0.868 | 5.157 | 1.00 | 0.00 H |
| ATOM | 479 | HA | ILE A | 36146.727 | 2.079 | 3.596 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.538 | 3.502 | 5.114 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.482 | 2.233 | 2.367 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.601 | 1.671 | 3.784 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36145.386 | 4.447 | 2.465 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36146.597 | 4.602 | 3.738 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36145.013 | 5.354 | 3.931 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36142.347 | 3.036 | 2.018 | 1.00 | 0.00 H |
| ATOM | 487 | 2HD1 | ILE A | 36143.183 | 4.428 | 2.706 | 1.00 | 0.00 H |
| ATOM | 488 | 3HD1 | ILE A | 36142.116 | 3.452 | 3.716 | 1.00 | 0.00 H |
| ATOM | 489 | N | ARGA | 37148.237 | 3.449 | 5.019 | 1.00 | 0.00 N |
| ATOM | 490 | $\mathbf{C}_{\mathbf{A}}$ | ARG A | 37149.215 | 4.113 | 5.872 | 1.00 | 0.00 C |
| ATOM | 491 | C | ARG A | 37149.395 | 5.571 | 5.462 | 1.00 | 0.00 C |
| ATOM | 492 | О | ARG A | 37149.097 | 6.483 | 6.232 | 1.00 | 0.00 O |
| ATOM | 493 | CB | ARG A | 37150.558 | 3.383 | 5.807 | 1.00 | 0.00 C |
| ATOM | 494 | CG | ARG A | 37150.462 | 1.902 | 6.127 | 7 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | 37149.957 | 1.669 | 7.543 | 3 1.00 | 0.00 C |
| ATOM | 496 | NE | ARG A | 37150.921 | 2.111 | 8.547 | 1.00 | 0.00 N |
| ATOM | 497 | CZ | ARG A | 37150.615 | 2.326 | 9.825 | 1.00 | 0.00 C |
| ATOM | 498 | NH1 | ARG A | 37149.373 | 2.142 | 10.257 | 1.00 | 0.00 N |

| ATOM | 499 | NH2 | ARG A | 37151.552 | 2.726 | 10.673 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 500 | Н | ARG A | 37148.412 | 3.377 | 4.057 | 1.00 | 0.00 H |
| ATOM | 501 | HA | ARG A | 37148.847 | 4.080 | 6.887 | 1.00 | 0.00 H |
| ATOM | 502 | 1HB | ARG A | 37150.964 | 3.489 | 4.811 | 1.00 | 0.00 H |
| ATOM | 503 2 | 2HB | ARG A | 37151.237 | 3.839 | 6.513 | 1.00 | 0.00 H |
| ATOM | 504 | 1HG | ARG A | 37149.779 | 1.436 | 5.432 | 1.00 | 0.00 H |
| ATOM | 505 2 | 2HG | ARG A | 37151.441 | 1.457 | 6.027 | 1.00 | 0.00 H |
| ATOM | 506 | 1HD | ARG A | 37149.036 | 2.217 | 7.676 | 1.00 | 0.00 H |
| ATOM | 507 2 | 2HD | ARG A | 37149.770 | 0.614 | 7.675 | 1.00 | 0.00 H |
| ATOM | 508 | HE | ARG A | 37151.845 | 2.255 | 8.255 | 1.00 | 0.00 H |
| ATOM | 509 | 1HH1 | ARG A | 37148.661 | 1.839 | 9.623 | 1.00 | 0.00 H |
| ATOM | 510 2 | 2HH1 | ARG A | 37149.150 | 2.304 | 11.218 | 1.00 | 0.00 H |
| ATOM | 511 | 1HH2 | ARG A | 37152.488 | 2.866 | 10.352 | 1.00 | 0.00 H |
| ATOM | 512 2 | 2HH2 | ARG A | 37151.322 | 2.887 | 11.632 | 1.00 | 0.00 H |
| ATOM | 513 | N | TRP A | 38149.882 | 5.784 | 4.244 | 1.00 | 0.00 N |
| ATOM | 514 | CA | TRP A | 38150.100 | 7.132 | 3.733 | 1.00 | 0.00 C |
| ATOM | 515 | C | TRP A | 38149.375 | 7.336 | 2.406 | 1.00 | 0.00 C |
| ATOM | 516 | О | TRPA | 38149.482 | 6.516 | 1.495 | 1.00 | 0.00 O |
| ATOM | 517 | СВ | TRPA | 38151.599 | 7.402 | 3.559 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38151.898 | 8.654 | 2.788 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRP A | 38152.099 | 9.904 | 3.297 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRP A | 38152.022 | 8.774 | 1.366 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRPA | 38152.341 | 10.795 | 2.279 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.299 | 10.126 | 1.084 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38151.926 | 7.871 | 0.304 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRPA | 38152.481 | 10.593 | -0.216 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.107 | 8.335 | -0.985 | 1.00 | 0.00 C |

| ATOM | 526 | CH2 | TRP A | 38152.381 | 9.685 | -1.236 | 1.00 | 0.00 C |
|--------|--------------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 527 | Н | TRP A | 38150.101 | 5.016 | 3.675 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRPA | 38149.700 | 7.828 | 4.456 | 1.00 | 0.00 H |
| ATOM | 529 1 | НВ | TRP A | 38152.056 | 7.494 | 4.533 | 1.00 | 0.00 H |
| ATOM | 530 2 | 2HB | TRPA | 38152.049 | 6.571 | 3.035 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38152.068 | 10.144 | 4.350 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38152.516 | 11.753 | 2.391 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRPA | 38151.715 | 6.827 | 0.477 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38152.690 | 11.631 | -0.427 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.037 | 7.652 | -1.818 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRP A | 38152.516 | 10.004 | -2.259 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.646 | 8.442 | 2.303 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39147.911 | 8.766 | 1.088 | 1.00 | 0.00 C |
| ATOM - | 539 | C | ILE A | 39148.340 | 10.125 | 0.546 | 1.00 | 0.00 C |
| ATOM | 540 | O | ILE A | 39147.988 | 11.165 | 1.104 | 1.00 | 0.00 O |
| ATOM | 541 | CB | ILE A | 39146.391 | 8.780 | 1.335 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39145.961 | 7.521 | 2.089 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.640 | 8.896 | 0.016 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.572 | 7.613 | 2.680 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.608 | 9.060 | 3.063 | 1.00 | 0.00 H |
| ATOM | 546 | НА | ILE A | 39148.130 | 8.008 | 0.350 | 1.00 | 0.00 H |
| ATOM | 547 | НВ | ILE A | 39146.153 | 9.647 | 1.932 | 1.00 | 0.00 H |
| ATOM | 548 1 | HG1 | ILE A | 39145.977 | 6.680 | 1.411 | 1.00 | 0.00 H |
| ATOM | 549 2 | 2HG1 | ILE A | 39146.656 | 7.338 | 2.897 | 1.00 | 0.00 H |
| ATOM | 550 1 | HG2 | ILE A | 39144.577 | 8.847 | 0.202 | 1.00 | 0.00 H |
| ATOM | 551 2 | 2HG2 | ILE A | 39145.930 | 8.085 | -0.636 | 1.00 | 0.00 H |
| ATOM | 552 3 | 3HG2 | ILE A | 39145.880 | 9.839 | -0.453 | 1.00 | 0.00 H |

| ATOM | 553 1H | HD1 | ILE A | 39143.973 | 8.287 | 2.086 | 1.00 | 0.00 H |
|------|--------|-----------------|-------|-----------|--------|--------|------|--------|
| ATOM | 554 2F | I D1 | ILE A | 39144.635 | 7.984 | 3.692 | 1.00 | 0.00 H |
| ATOM | 555 3H | HD1 | ILE A | 39144.116 | 6.634 | 2.682 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.108 | 10.112 | -0.539 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.576 | 11.353 | -1.126 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.128 | 11.169 | -2.526 | 1.00 | 0.00 C |
| ATOM | 559 | O | GLY A | 40149.973 | 10.107 | -3.129 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.362 | 9.254 | -0.940 | 1.00 | 0.00 H |
| ATOM | 561 1H | ŀΑ | GLY A | 40148.755 | 12.052 | -1.165 | 1.00 | 0.00 H |
| ATOM | 562 2H | ΙA | GLY A | 40150.351 | 11.763 | -0.498 | 1.00 | 0.00 H |
| ATOM | 563 | Ν | GLN A | 41150.772 | 12.210 | -3.042 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.352 | 12.170 | -4.378 | 1.00 | 0.00 C |
| ATOM | 565 | C , | GLN A | 41152.824 | 12.581 | -4.341 | 1.00 | 0.00 C |
| ATOM | 566 | О | GLN A | 41153.146 | 13.724 | -4.012 | 1.00 | 0.00 O |
| ATOM | 567 | СВ | GLN A | 41150.574 | 13.098 | -5.310 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41149.068 | 12.908 | -5.240 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.312 | 14.221 | -5.293 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.274 | 14.968 | -4.315 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41147.705 | 14.509 | -6.437 | 1.00 | 0.00 N |
| ATOM | 572 | H | GLN A | 41150.861 | 13.027 | -2.510 | 1.00 | 0.00 H |
| ATOM | 573 | HA | GLN A | 41151.277 | 11.159 | -4.745 | 1.00 | 0.00 H |
| ATOM | 574 1H | ·IB | GLN A | 41150.798 | 14.121 | -5.048 | 1.00 | 0.00 H |
| ATOM | 575 2H | ·Β | GLN A | 41150.892 | 12.919 | -6.325 | 1.00 | 0.00 H |
| ATOM | 576 1H | łG | GLN A | 41148.754 | 12.298 | -6.074 | 1.00 | 0.00 H |
| ATOM | 577 2H | łG | GLN A | 41148.824 | 12.406 | -4.316 | 1.00 | 0.00 H |
| ATOM | 578 1H | HE2 | GLN A | 41147.778 | 13.866 | -7.174 | 1.00 | 0.00 H |
| ATOM | 579 2H | HE2 | GLN A | 41147.211 | 15.351 | -6.500 | 1.00 | 0.00 H |

| ATOM | 580 N | PRO A | 42153.742 | 11.656 | -4.675 | 1.00 | 0.00 N |
|------|---------|-------|-----------|--------|---------|------|--------|
| ATOM | 581 CA | PRO A | 42155.181 | 11.939 | -4.673 | 1.00 | 0.00 C |
| ATOM | 582 C | PRO A | 42155.542 | 13.108 | -5.584 | 1.00 | 0.00 C |
| ATOM | 583 O | PRO A | 42154.782 | 13.461 | -6.486 | 1.00 | 0.00 O |
| ATOM | 584 CB | PRO A | 42155.808 | 10.641 | -5.194 | 1.00 | 0.00 C |
| ATOM | 585 CG | PRO A | 42154.786 | 9.590 | -4.928 | 1.00 | 0.00 C |
| ATOM | 586 CD | PRO A | 42153.455 | 10.268 | -5.079 | 1.00 | 0.00 C |
| ATOM | 587 HA | PRO A | 42155.542 | 12.139 | -3.674 | 1.00 | 0.00 H |
| ATOM | 588 1HB | PRO A | 42156.012 | 10.737 | -6.250 | 1.00 | 0.00 H |
| ATOM | 589 2HB | PRO A | 42156.725 | 10.442 | -4.661 | 1.00 | 0.00 H |
| ATOM | 590 1HG | PRO A | 42154.883 | 8.791 | -5.647 | 1.00 | 0.00 H |
| ATOM | 591 2HG | PRO A | 42154.901 | 9.210 | -3.923 | 1.00 | 0.00 H |
| ATOM | 592 1HD | PRO A | 42153.124 | 10.226 | -6.107 | 1.00 | 0.00 H |
| ATOM | 593 2HD | PRO A | 42152.724 | 9.819 | -4.424 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43156.714 | 13.726 | -5.360 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.174 | 14.860 | -6.166 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43157.596 | 14.441 | -7.569 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43158.768 | 14.155 | -7.816 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43158.377 | 15.386 | - 5.384 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43158.887 | 14.204 | -4.634 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43157.681 | 13.366 | -4.305 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43156.419 | 15.630 | -6.233 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43159.117 | 15.767 | -6.073 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43158.061 | 16.171 | -4.714 | 1.00 | 0.00 H |
| ATOM | 604 1HG | PRO A | 43159.573 | 13.646 | -5.253 | 1.00 | 0.00 H |
| ATOM | 605 2HG | PRO A | 43159.376 | 14.528 | -3.728 | 1.00 | 0.00 H |
| ATOM | 606 1HD | PRO A | 43157.928 | 12.316 | -4.350 | 1.00 | 0.00 H |

| ATOM | 607 2HD | PRO A | 43157.298 | 13.624 | -3.329 | 1.00 | 0.00 H |
|------|----------|---------|-----------|----------|---------|------|--------|
| ATOM | 608 N | GLY A | 44156.635 | 14.406 | -8.486 | 1.00 | 0.00 N |
| ATOM | 609 CA | GLY A | 44156.931 | 14.021 | -9.852 | 1.00 | 0.00 C |
| ATOM | 610 C | GLY A | 44155.710 | 13.511 - | 10.590 | 1.00 | 0.00 C |
| ATOM | (611 O | GLY A | 44155.412 | 13.962 - | -11.696 | 1.00 | 0.00 O |
| ATOM | 612 H | GLY A | 44155.719 | 14.645 | -8.232 | 1.00 | 0.00 H |
| ATOM | 613 1HA | GLY A | 44157.323 | 14.877 - | 10.378 | 1.00 | 0.00 H |
| ATOM | 614 2HA | GLY A | 44157.681 | 13.245 | -9.840 | 1.00 | 0.00 H |
| ATOM | 615 N | LEU A | 45155.002 | 12.568 | -9.979 | 1.00 | 0.00 N |
| ATOM | 616 CA | LEU A | 45153.807 | 11.996 | -10.589 | 1.00 | 0.00 C |
| ATOM | 617 C | LEU A | 45152.592 | 12.203 | -9.694 | 1.00 | 0.00 C |
| ATOM | 618 O | LEU A | 45152.501 | 11.623 | -8.612 | 1.00 | 0.00 O |
| ATOM | 619 CB | LEU A | 45154.011 | 10.504 | -10.858 | 1.00 | 0.00 C |
| ATOM | 620 CG | LEU A | 45154.560 | 9.704 | -9.674 | 1.00 | 0.00 C |
| ATOM | 621 CD | 1 LEU A | 45154.219 | 8.227 | -9.821 | 1.00 | 0.00 C |
| ATOM | 622 CD | 2 LEU A | 45156.066 | 9.899 | -9.551 | 1.00 | 0.00 C |
| ATOM | 623 H | LEU A | 45155.289 | 12.247 | -9.096 | 1.00 | 0.00 H |
| ATOM | 624 HA | LEU A | 45153.640 | 12.503 | -11.528 | 1.00 | 0.00 H |
| ATOM | 625 1HB | LEU A | 45153.060 | 10.079 - | 11.144 | 1.00 | 0.00 H |
| ATOM | 626 2HB | LEU A | 45154.698 | 10.399 - | 11.684 | 1.00 | 0.00 H |
| ATOM | 627 HG | LEU A | 45154.101 | 10.062 | -8.764 | 1.00 | 0.00 H |
| ATOM | 628 1HD | I LEU A | 45153.622 | 8.081 - | 10.710 | 1.00 | 0.00 H |
| ATOM | 629 2HD | I LEU A | 45153.661 | 7.900 | -8.956 | 1.00 | 0.00 H |
| ATOM | 630 3HD | I LEU A | 45155.130 | 7.652 | -9.900 | 1.00 | 0.00 H |
| ATOM | 631 1HD2 | 2 LEU A | 45156.572 | 8.983 | -9.824 | 1.00 | 0.00 H |
| ATOM | 632 2HD2 | 2 LEU A | 45156.312 | 10.155 | -8.530 | 1.00 | 0.00 H |
| ATOM | 633 3HD | 2 LEU A | 45156.383 | 10.694 - | 10.208 | 1.00 | 0.00 H |

| ATOM | 634 | N | ASN A | 46151.656 | 13.030 | -10.149 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|----------|---------|------|--------|
| ATOM | 635 | CA | ASN A | 46150.449 | 13.299 | -9.377 | 1.00 | 0.00 C |
| ATOM | 636 | С | ASN A | 46149.512 | 12.098 | -9.414 | 1.00 | 0.00 C |
| ATOM | 637 | Ο | ASN A | 46148.893 | 11.810 | -10.438 | 1.00 | 0.00 O |
| ATOM | 638 | СВ | ASN A | 46149.736 | 14.537 | -9.925 | 1.00 | 0.00 C |
| ATOM | 639 | CG | ASN A | 46148.974 | 15.289 | -8.852 | 1.00 | 0.00 C |
| ATOM | 640 | OD1 | ASN A | 46147.746 | 15.375 | -8.891 | 1.00 | 0.00 O |
| ATOM | 641 | ND2 | ASN A | 46149.700 | 15.838 | -7.884 | 1.00 | 0.00 N |
| ATOM | 642 | Н | ASN A | 46151.778 | 13.465 | -11.018 | 1.00 | 0.00 H |
| ATOM | 643 | HA | ASN A | 46150.742 | 13.484 | -8.355 | 1.00 | 0.00 H |
| ATOM | 644 | lНВ | ASN A | 46150.466 | 15.205 - | 10.356 | 1.00 | 0.00 H |
| ATOM | 645 2 | 2HB | ASN A | 46149.038 | 14.232 - | 10.691 | 1.00 | 0.00 H |
| ATOM | 646 | HD2 | ASN A | 46150.673 | 15.727 | -7.917 | 1.00 | 0.00 H |
| ATOM | 647 2 | 2HD2 | ASN A | 46149.233 | 16.329 | -7.178 | 1.00 | 0.00 H |
| ATOM | 648 | N | GLU A | 47149.415 | 11.401 | -8.288 | 1.00 | 0.00 N |
| ATOM | 649 | CA | GLU A | 47148.555 | . 10.230 | -8.183 | 1.00 | 0.00 C |
| ATOM | 650 | С | GLU A | 47148.375 | 9.820 | -6.726 | 1.00 | 0.00 C |
| ATOM | 651 | О | GLU A | 47149.348 | 9.519 | -6.034 | 1.00 | 0.00 O |
| ATOM | 652 | СВ | GLU A | 47149.138 | 9.063 | -8.985 | 1.00 | 0.00 C |
| ATOM | 653 | CG | GLU A | 47150.653 | 8.959 | -8.902 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.235 | 8.068 | -9.981 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.350 | 8.531 - | 11.134 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.575 | 6.905 | -9.672 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47149.935 | 11.682 | -7.507 | 1.00 | 0.00 H |
| ATOM | 658 | НА | GLU A | 47147.590 | 10.490 | -8.592 | 1.00 | 0.00 H |
| ATOM | 659 | IHB | GLU A | 47148.715 | 8.141 | -8.616 | 1.00 | 0.00 H |
| ATOM | 660 2 | 2HB | GLU A | 47148.864 | 9.183 | -10.022 | 1.00 | 0.00 H |

| ATOM | 661 | 1HG | GLU A | 47151.075 | 9.946 | -9.006 | 1.00 | 0.00 H |
|-------------------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 662 | 2HG | GLU A | 47150.922 | 8.554 | -7.937 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.130 | 9.802 | -6.264 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VAL A | 48146.839 | 9.420 | -4.889 | 1.00 | 0.00 C |
| ATOM | 665 | C | VALA | 48147.232 | 7.969 | -4.639 | 1.00 | 0.00 C |
| ATOM | 666 | O | VAL A | 48146.502 | 7.047 | -5.001 | 1.00 | 0.00 O |
| ATOM | 667 | СВ | VAL A | 48145.346 | 9.605 | -4.557 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VAL A | 48145.100 | 9.395 | -3.071 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VALA | 48144.867 | 10.980 | -4.996 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.393 | 10.047 | -6.862 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.417 | 10.058 | -4.236 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48144.783 | 8.860 | -5.100 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48144.082 | 9.666 | -2.834 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VAL A | 48145.780 | 10.014 | -2.503 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48145.265 | 8.358 | -2.821 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48145.704 | 11.662 | -5.017 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48144.125 | 11.342 | -4.301 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VAL A | 48144.433 | 10.912 | -5.983 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.392 | 7.774 | -4.021 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49148.884 | 6.434 | -3.727 | 1.00 | 0.00 C |
| ATOM | 681 | C | LEU A | 49148.782 | 6.135 | -2.237 | 1.00 | 0.00 C |
| ATOM | 682 | О | LEU A | 49149.437 | 6.780 | -1.418 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.333 | 6.286 | -4.190 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.544 | 6.396 | -5.702 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49151.921 | 6.965 | -6.009 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEU A | 49150.367 | 5.038 | -6.363 | 1.00 | 0.00 C |
| ATOM [,] | 687 | Н | LEU A | 49148.932 | 8.549 | -3.758 | 1.00 | 0.00 H |

| ATOM | 688 HA | LEU A | 49148.269 | 5.729 | -4.266 | 1.00 | 0.00 H |
|------|----------|-------|-----------|-------|--------|------|--------|
| ATOM | 689 1HB | LEU A | 49150.924 | 7.053 | -3.709 | 1.00 | 0.00 H |
| ATOM | 690 2HB | LEU A | 49150.696 | 5.322 | -3.869 | 1.00 | 0.00 H |
| ATOM | 691 HG | LEU A | 49149.806 | 7.068 | -6.114 | 1.00 | 0.00 H |
| ATOM | 692 1HD1 | LEU A | 49151.845 | 8.033 | -6.150 | 1.00 | 0.00 H |
| ATOM | 693 2HD1 | LEU A | 49152.306 | 6.509 | -6.908 | 1.00 | 0.00 H |
| ATOM | 694 3HD1 | LEU A | 49152.588 | 6.757 | -5.186 | 1.00 | 0.00 H |
| ATOM | 695 1HD2 | LEU A | 49151.056 | 4.331 | -5.924 | 1.00 | 0.00 H |
| ATOM | 696 2HD2 | LEU A | 49150.566 | 5.123 | -7.421 | 1.00 | 0.00 H |
| ATOM | 697 3HD2 | LEU A | 49149.354 | 4.694 | -6.214 | 1.00 | 0.00 H |
| ATOM | 698 N | ALA A | 50147.954 | 5.157 | -1.890 | 1.00 | 0.00 N |
| ATOM | 699 CA | ALAA | 50147.767 | 4.778 | -0.498 | 1.00 | 0.00 C |
| ATOM | 700 C | ALA A | 50148.728 | 3.663 | -0.099 | 1.00 | 0.00 C |
| ATOM | 701 O | ALA A | 50148.645 | 2.546 | -0.611 | 1.00 | 0.00 O |
| ATOM | 702 CB | ALA A | 50146.329 | 4.352 | -0.254 | 1.00 | 0.00 C |
| ATOM | 703 H | ALA A | 50147.457 | 4.680 | -2.588 | 1.00 | 0.00 H |
| ATOM | 704 HA | ALA A | 50147.968 | 5.649 | 0.110 | 1.00 | 0.00 H |
| ATOM | 705 1HB | ALA A | 50146.304 | 3.578 | 0.500 | 1.00 | 0.00 H |
| ATOM | 706 2HB | ALA A | 50145.905 | 3.973 | -1.172 | 1.00 | 0.00 H |
| ATOM | 707 3HB | ALA A | 50145.753 | 5.201 | 0.084 | 1.00 | 0.00 H |
| ATOM | 708 N | GLY A | 51149.639 | 3.971 | 0.818 | 1.00 | 0.00 N |
| ATOM | 709 CA | GLY A | 51150.601 | 2.984 | 1.269 | 1.00 | 0.00 C |
| ATOM | 710 C | GLY A | 51149.968 | 1.910 | 2.133 | 1.00 | 0.00 C |
| ATOM | 711 O | GLY A | 51149.673 | 2.142 | 3.305 | 1.00 | 0.00 O |
| ATOM | 712 H | GLY A | 51149.657 | 4.877 | 1.191 | 1.00 | 0.00 H |
| ATOM | 713 1HA | GLY A | 51151.053 | 2.516 | 0.406 | 1.00 | 0.00 H |
| ATOM | 714 2HA | GLY A | 51151.371 | 3.482 | 1.839 | 1.00 | 0.00 H |

| ATOM | 715 | N | LEU A | 52149.760 | 0.733 | 1.554 | 1.00 | 0.00 N |
|------|-------------|------|-------|-----------|---------|--------|------|----------|
| ATOM | 716 | CA | LEU A | 52149.158 | -0.379 | 2.279 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.226 | -1.227 | 2.962 | 1.00 | 0.00 C |
| ATOM | 718 | Ο | LEU A | 52151.311 | -1.435 | 2.418 | 1.00 | 0.00 O |
| ATOM | 719 | СВ | LEU A | 52148.331 | -1.247 | 1.329 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.092 | -0.567 | 0.742 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.492 | -1.417 | -0.367 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEUA | 52146.064 | -0.305 | 1.832 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.018 | 0.609 | 0.617 | 1.00 | 0.00 H |
| ATOM | 724 | HA | LEU A | 52148.505 | 0.033 | 3.035 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.968 | -1.558 | 0.513 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52148.010 | -2.127 | 1.866 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.380 | 0.383 | 0.317 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52146.896 | -1.104 | -1.319 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52145.420 | -1.294 | -0.374 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52146.736 | - 2.456 | -0.197 | 1.00 | 0.00 H |
| ATOM | 73 1 | 1HD2 | LEU A | 52146.171 | -1.044 | 2.613 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52145.071 | -0.367 | 1.412 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52146.220 | 0.680 | 2.245 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53149.911 | -1.716 | 4.157 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.842 | -2.542 | 4.916 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.337 | -3.977 | 5.018 | 1.00 | 0.00 C |
| ATOM | 737 | О | GLU A | 53149.366 | -4.256 | 5.720 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.049 | -1.961 | 6.316 | 1.00 | . 0.00 C |
| ATOM | 739 | CG | GLU A | 53152.034 | -2.750 | 7.163 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.587 | -2.881 | 8.606 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53152.298 | -2.368 | 9.497 | 1.00 | 0.00 O |

| ATOM | 742 | OE2 | GLU A | 53150.528 | -3.497 | 8.845 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|--------|--------|------|---------------------|
| ATOM | 743 | Н | GLU A | 53149.031 | -1.515 | 4.539 | 1.00 | 0.00 H |
| ATOM | 744 | НА | GLU A | 53151.787 | -2.541 | 4.393 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.416 | -0.950 | 6.224 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53150.099 | -1.944 | 6.830 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53152.138 | -3.739 | 6.743 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53152.990 | -2.248 | 7.141 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54151.003 | -4.885 | 4.310 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.620 | -6.292 | 4.319 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54150.836 | -6.904 | 5.700 | 1.00 | 0.00 C |
| ATOM | 752 | Ο | LEU A | 54151.871 | -6.692 | 6.329 | 1.00 | 0.00 O |
| ATOM | 753 | CB | LEU A | 54151.423 | -7.067 | 3.273 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.413 | -6.460 | 1.869 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.554 | -7.023 | 1.036 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54150.076 | -6.717 | 1.189 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.769 | -4.601 | 3.768 | 1.00 | 0.00 H |
| ATOM | 758 | HA | LEU A | 54149.571 | -6.352 | 4.072 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.448 | -7.128 | 3.610 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54151.022 | -8.068 | 3.211 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.551 | -5.392 | 1.944 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54152.684 | -8.071 | 1.266 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54153.463 | -6.489 | 1.263 | 1.00 | 0.00 ³ H |
| ATOM | 764 | 3HD1 | LEU A | 54152.323 | -6.911 | -0.013 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54149.629 | -7.612 | 1.599 | 1.00 | 0.00 H |
| ATOM | 766 | 2HD2 | LEU A | 54150.230 | -6.846 | 0.128 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.419 | -5.877 | 1.357 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55149.850 | -7.665 | 6.164 | 1.00 | 0.00 N |

| ATOM | 769 | CA | GLU A | 55149.930 | -8.310 | 7.469 | 1.00 | 0.00 C |
|------|--------------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 770 | C | GLU A | 55151.044 | -9.351 | 7.494 | 1.00 | 0.00 C |
| ATOM | 771 | O | GLU A | 55151.685 | -9.565 | 8.524 | 1.00 | 0.00 O |
| ATOM | 772 | СВ | GLU A | 55148.594 | -8.967 | 7.822 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55147.552 | -7.987 | 8.337 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55146.137 | -8.398 | 7.975 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55145.968 | -9.127 | 6.975 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55145.200 | -7.990 | 8.692 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.048 | -7.797 | 5.615 | 1.00 | 0.00 H |
| ATOM | 778 | НА | GLU A | 55150.150 | -7.547 | 8.202 | 1.00 | 0.00 H |
| ATOM | 779 1 | НВ | GLU A | 55148.199 | -9.448 | 6.939 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55148.763 | -9.712 | 8.584 | 1.00 | 0.00 H |
| ATOM | 781 1 | HG | GLU A | 55147.630 | -7.930 | 9.412 | 1.00 | 0.00 H |
| ATOM | 782 2 | HG | GLU A | 55147.749 | -7.015 | 7.910 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56151.269 | -9.997 | 6.356 | 1.00 | 0.00 Ņ |
| ATOM | 784 | CA | ASPA | 56152.306 | -11.017 | 6.248 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASP A | 56153.580 - | 10.435 | 5.642 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASPA | 56153.529 | -9.483 | 4.864 | 1.00 | 0.00 O |
| ATOM | 787 | СВ | ASPA | 56151.812 | -12.189 | 5.397 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56150.930 | -13.140 | 6.180 | 1.00 | 0.00 C |
| ATOM | 7.89 | OD1 | ASPA | 56149.691 - | 13.034 | 6.064 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56151.478 - | 13.993 | 6.910 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.725 | -9.784 | 5.569 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.526 | -11.374 | 7.243 | 1.00 | 0.00 H |
| ATOM | 793 1 | HB | ASPA | 56151.244 - | -11.805 | 4.563 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASPA | 56152.664 - | 12.739 | 5.024 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.719 | -11.014 | 6.006 | 1.00 | 0.00 N |

| ATOM | 796 | CA | GLU A | 57156.006 - | -10.552 | 5.498 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|--------|------|---------|
| ATOM | 797 | С | GLU A | 57156.353 - | 11.245 | 4.184 | 1.00 | 0.00 C |
| ATOM | 798 | Ο | GLU A | 57156.738 - | 12.414 | 4.170 | 1.00 | 0.00 O |
| ATOM | 799 | СВ | GLU A | 57157.107 - | 10.810 | 6.529 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.130 | -9.795 | 7.660 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57158.393 | -9.882 | 8.496 | 1.00 | .0.00 C |
| ATOM | 802 | OE1 | GLU A | 57158.992 - | 10.976 | 8.553 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57158.782 | -8.856 | 9.092 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.694 - | 11.769 | 6.630 | 1.00 | 0.00 H |
| ATOM | 805 | НА | GLU A | 57155.932 | -9.490 | 5.323 | 1.00 | 0.00 H |
| ATOM | 806 1 | НВ | GLU A | 57156.960 - | 11.791 | 6.958 | 1.00 | 0.00 H |
| ATOM | 807 2 | HB | GLU A | 57158.064 - | 10.784 | 6.031 | 1.00 | 0.00 H |
| ATOM | 808 1 | HG | GLU A | 57157.065 | -8.803 | 7.238 | 1.00 | 0.00 H |
| ATOM | 809 2 | HG | GLU A | 57156.278 | -9.969 | 8.301 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58156.214 - | 10.515 | 3.082 | 1.00 | 0.00 N |
| ATOM | 811 | CA | CYS A | 58156.513 - | 11.058 | 1.762 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58157.824 - | 10.492 | 1.225 | 1.00 | 0.00 C |
| ATOM | 813 | O | CYS A | 58157.973 | -9.279 | 1.077 | 1.00 | 0.00 O |
| ATOM | 814 | СВ | CYS A | 58155.374 - | 10.750 | 0.790 | 1.00 | 0.00 C |
| ATOM | 815 | SG | CYS A | 58155.604 - | 11.445 | -0.862 | 1.00 | 0.00 S |
| ATOM | 816 | H | CYS A | 58155.904 | -9.589 | 3.158 | 1.00 | 0.00 H |
| ATOM | 817 | НА | CYSA | 58156.612 - | 12.129 | 1.860 | 1.00 | 0.00 H |
| ATOM | 818 1 | HB | CYS A | 58154.453 - | 11.150 | 1.188 | 1.00 | 0.00 H |
| ATOM | 819 2 | HB | CYS A | 58155.279 | -9.678 | 0.687 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYS A | 58156.540 - | -11.627 | -0.979 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALA A | 59158.770 - | 11.378 | 0.933 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALAA | 59160.067 - | 10.966 | 0.411 | 1.00 | 0.00 C |

| ATOM | 823 | C | ALAA | 59159.915 - | 10.208 | -0.903 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 824 | O | ALAA | 59159.155 - | 10.615 | -1.782 | 1.00 | 0.00 O |
| ATOM | 825 | СВ | ALA A | 59160.968 | -12.177 | 0.223 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALAA | 59158.592 - | 12.331 | 1.071 | 1.00 | 0.00 H |
| ATOM | 827 | НА | ALA A | 59160.528 | -10.315 | 1.140 | 1.00 | 0.00 H |
| ATOM | 828 | 1HB | ALA A | 59160.734 - | 12.921 | 0.969 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59162.001 - | 11.877 | 0.326 | 1.00 | 0.00 H |
| ATOM | 830 3 | ЗНВ | ALA A | 59160.811 - | 12.593 | -0.762 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60160.643 | -9.103 | -1.031 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60160.574 | -8.305 | -2.241 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60160.044 | -6.908 | -1.985 | 1.00 | 0.00 C |
| ATOM | 834 | O | GLY A | 60160.381 | -5.967 | -2.703 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60161.231 | -8.827 | -0.298 | 1.00 | 0.00 H |
| ATOM | 836 | ΙHΑ | GLY A | 60161.564 | -8.229 | -2.666 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60159.927 | -8.799 | -2.951 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61159.210 | -6.773 | -0.959 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.631 | -5.480 | -0.610 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.598 | -4.662 | 0.240 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.705 | -5.109 | 0.542 | 1.00 | 0.00 O |
| ATOM | 842 | СВ | CYS A | 61157.314 | -5.675 | 0.143 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYS A | 61156.183 | -6.848 | -0.641 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.978 | -7.560 | -0.424 | 1.00 | 0.00 H |
| ATOM | 845 | HA | CYS A | 61158.435 | -4.946 | -1.527 | 1.00 | 0.00 H |
| ATOM | 846 | HB | CYS A | 61157.525 | -6.040 | 1.137 | 1.00 | 0.00 H |
| ATOM | 847 2 | 2НВ | CYS A | 61156.804 | -4.725 | 0.215 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61156.528 | -7.057 | -1.512 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62159.174 | -3.462 | 0.620 | 1.00 | 0.00 N |

| ATOM | 850 | CA | THR A | 62160.003 | -2.581 | 1.435 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 851 | C | THR A | 62159.434 | -2.448 | 2.844 | 1.00 | 0.00 C |
| ATOM | 852 | О | THR A | 62158.454 | -3.106 | 3.192 | 1.00 | 0.00 O |
| ATOM | 853 | СВ | THR A | 62160.110 | -1.201 | 0.784 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.839 | -0.580 | 0.714 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.677 | -1.243 | -0.618 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62158.283 | -3.161 | 0.347 | 1.00 | 0.00 H |
| ATOM | 857 | НА | THR A | 62160.989 | -3.017 | 1.497 | 1.00 | 0.00 H |
| ATOM | 858 | НВ | THR A | 62160.758 | -0.580 | 1.385 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62158.243 | -1.125 | 0.195 | 1.00 | 0.00 H |
| ATOM | 860 1 | HG2 | THR A | 62160.591 | -2.245 | -1.011 | 1.00 | 0.00 H |
| ATOM | 861 2 | 2HG2 | THR A | 62161.718 | -0.954 | -0.595 | 1.00 | 0.00 H |
| ATOM | 862 3 | 3HG2 | THR A | 62160.128 | -0.561 | -1.250 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63160.056 | -1.594 | 3.649 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASPA | 63159.612 | -1.375 | 5.021 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.866 | -0.050 | 5.147 | 1.00 | 0.00 C |
| ATOM | 866 | O | ASPA | 63158.935 | 0.616 | 6.180 | 1.00 | 0.00 O |
| ATOM | 867 | СВ | ASPA | 63160.806 | -1.393 | 5.976 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.904 | -0.439 | 5.547 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63162.936 | -0.917 | 5.028 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63161.732 | 0.784 | 5.729 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASPA | 63160.832 | -1.098 | 3.314 | 1.00 | 0.00 H |
| ATOM | 872 | НА | ASPA | 63158.940 | -2.178 | 5.284 | 1.00 | 0.00 H |
| ATOM | 873 1 | lНВ | ASPA | 63160.475 | -1.110 | 6.963 | 1.00 | 0.00 H |
| ATOM | 874 2 | 2HB | ASPA | 63161.216 | -2.393 | 6.011 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64158.156 | 0.325 | 4.089 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.408 | 1.569 | 4.101 | 1.00 | 0.00 C |

| ATOM | 877 | C | GLY A | 64158.144 | 2.695 | 3.402 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 878 | О | GLY A | 64158.130 | 3.836 | 3.864 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64158.138 | -0.246 | 3.293 | 1.00 | 0.00 H |
| ATOM | 880 | 1HA | GLY A | 64156.460 | 1.412 | 3.608 | 1.00 | 0.00 H |
| ATOM | 881 2 | 2HA | GLY A | 64157.225 | 1.856 | 5.126 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.787 | 2.375 | 2.284 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.532 | 3.367 | 1.519 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65159.121 | 3.343 | 0.051 | 1.00 | 0.00 C |
| ATOM | 885 | Ο | THR A | 65159.276 | 2.330 | -0.631 | 1.00 | 0.00 O |
| ATOM | 886 | СВ | THR A | 65161.036 | 3.116 | 1.644 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.300 | 1.733 | 1.811 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.670 | 3.849 | 2.806 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.760 | 1.448 | 1.967 | 1.00 | 0.00 H |
| ATOM | 890 | HA | THR A | 65159.304 | 4.341 | 1.929 | 1.00 | 0.00 H |
| ATOM | 891 | НВ | THR A | 65161.522 | 3.447 | 0.738 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65161.736 | 1.394 | 1.027 | 1.00 | 0.00 H |
| ATOM | 893 | 1HG2 | THR A | 65161.388 | 3.369 | 3.731 | 1.00 | 0.00 H |
| ATOM | 894 2 | 2HG2 | THR A | 65161.331 | 4.874 | 2.813 | 1.00 | 0.00 H |
| ATOM | 895 | 3HG2 | THR A | 65162.745 | 3.826 | 2.702 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.597 | 4.466 | -0.431 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.164 | 4.572 | -1.819 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.235 | 5.243 | -2.672 | 1.00 | 0.00 C |
| ATOM | 899 | О | PHE A | 66159.380 | 6.465 | -2.657 | 1.00 | 0.00 O |
| ATOM | 900 | CB | PHE A | 66156.857 | 5.362 | -1.909 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.098 | 5.124 | -3.184 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.827 | 3.835 | -3.613 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.657 | 6.190 | -3.951 | 1.00 | 0.00 C |

| ATOM | 904 | CE1 | PHE A | 66155.130 | 3.613 | -4.786 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 905 | CE2 | PHE A | 66154.959 | 5.974 | -5.125 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.695 | 4.684 | -5.542 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.499 | 5.240 | 0.162 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66157.997 | 3.574 | -2.192 | 1.00 | 0.00 H |
| ATOM | 909 1 | НВ | PHE A | 66156.218 | 5.082 | -1.085 | 1.00 | 0.00 H |
| ATOM | 910 2 | НВ | PHE A | 66157.078 | 6.417 | -1.844 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66156.166 | 2.997 | -3.022 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66155.863 | 7.198 | -3.626 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66154.926 | 2.603 | -5.111 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66154.621 | 6.812 | -5.715 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.150 | 4.514 | -6.459 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.983 | 4.435 | -3.417 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67161.042 | 4.949 | -4.278 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67162.083 | 5.713 | -3.465 | 1.00 | 0.00 C |
| ATOM | 919 | O | ARG A | 67162.723 | 6.636 | -3.969 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67160.453 | 5.860 | -5.357 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67159.223 | 5.281 | -6.038 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67158.382 | 6.368 | -6.687 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67157.338 | 5.813 | -7.546 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67157.567 | 5.297 | -8.752 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67158.799 | 5.263 | -9.244 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67156.561 | 4.814 | -9.466 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.819 | 3.469 | -3.387 | 1.00 | 0.00 H |
| ATOM | 928 | НА | ARG A | 67161.521 | 4.107 | -4.753 | 1.00 | 0.00 H |
| ATOM | 929 1 | НВ | ARG A | 67160.177 | 6.802 | -4.906 | 1.00 | 0.00 H |
| ATOM | 930 2 | HB | ARG A | 67161.205 | 6.037 | -6.112 | 1.00 | 0.00 H |

| ATOM | 931 | lHG | ARG A | 67159.539 | 4.582 | -6.797 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 932 2 | 2HG | ARG A | 67158.623 | 4.768 | -5.300 | 1.00 | 0.00 H |
| ATOM | 933 | IHD | ARG A | 67157.919 | 6.959 | -5.910 | 1.00 | 0.00 H |
| ATOM | 934 2 | 2HD | ARG A | 67159.027 | 6.998 | -7.281 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67156.419 | 5.826 | -7.206 | 1.00 | 0.00 H |
| ATOM | 936 | IHH1 | ARG A | 67159.562 | 5.625 | -8.709 | 1.00 | 0.00 H |
| ATOM | 937 2 | 2HH1 | ARG A | 67158.964 | 4.873 - | 10.149 | 1.00 | 0.00 H |
| ATOM | 938 | HH2 | ARG A | 67155.630 | 4.837 | -9.101 | 1.00 | 0.00 H |
| ATOM | 939 2 | 2HH2 | ARG A | 67156.731 | 4.426 - | 10.372 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.246 | 5.323 | -2.205 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.211 | 5.983 | -1.344 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.572 | 7.006 | -0.425 | 1.00 | 0.00 C |
| ATOM | 943 | О | GLY A | 68163.149 | 7.375 | 0.598 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68161.708 | 4.581 | -1.856 | 1.00 | 0.00 H |
| ATOM | 945 | lНА | GLY A | 68163.709 | 5.237 | -0.743 | 1.00 | 0.00 H |
| ATOM | 946 2 | 2HA | GLY A | 68163.946 | 6.480 | -1.961 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.378 | 7.467 | -0.787 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.666 | 8.455 | 0.015 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69159.834 | 7.778 | 1.100 | 1.00 | 0.00 C |
| ATOM | 950 | О | THR A | 69158.714 | 7.331 | 0.851 | 1.00 | 0.00 O |
| ATOM | 951 | СВ | THR A | 69159.763 | 9.310 | -0.875 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.491 | 9.830 | -1.974 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69159.137 | 10.479 | -0.146 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.967 | 7.138 | -1.614 | 1.00 | 0.00 H |
| ATOM | 955 | HA | THR A | 69161.399 | 9.091 | 0.486 | 1.00 | 0.00 H |
| ATOM | 956 | HB | THR A | 69158.964 | 8.693 | -1.259 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.267 | 10.293 | -1.655 | 1.00 | 0.00 H |

| ATOM | 958 | 1HG2 | THR A | 69158.646 | 11.126 | -0.857 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 959 | 2HG2 | THR A | 69159.906 | 11.033 | 0.374 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69158.413 | 10.113 | 0.567 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.389 | 7.706 | 2.306 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.699 | 7.084 | 3.429 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.562 | 7.971 | 3.925 | 1.00 | 0.00 C |
| ATOM | 964 | O | ARG A | 70158.773 | 9.132 | 4.275 | 1.00 | 0.00 O |
| ATOM | 965 | СВ | ARG A | 70160.680 | 6.807 | 4.569 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70160.151 | 5.828 | 5.603 | 1.00 | 0.00 C |
| ATOM | 967 | CD | ARG A | 70160.885 | 5.964 | 6.927 | 1.00 | 0.00 C |
| ATOM | 968 | NE | ARG A | 70162.332 | 5.847 | 6.766 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70163.172 | 5.583 | 7.765 | 1.00 | 0.00 C |
| ATOM | 970 | NH1 | ARG A | 70162.711 | 5.408 | 8.998 | 1.00 | 0.00 N |
| ATOM | 971 | NH2 | ARG A | 70164.473 | 5.494 | 7.532 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.285 | 8.080 | 2.443 | 1.00 | 0.00 H |
| ATOM | 973 | НА | ARG A | 70159.286 | 6.147 | 3.086 | 1.00 | 0.00 H |
| ATOM | 974 | 1HB | ARG A | 70161.592 | 6.402 | 4.154 | 1.00 | 0.00 H |
| ATOM | 975 | 2HB | ARG A | 70160.906 | 7.738 | 5.069 | 1.00 | 0.00 H |
| ATOM | 976 | 1HG | ARG A | 70159.102 | 6.021 | 5.764 | 1.00 | 0.00 H |
| ATOM | 977 | 2HG | ARG A | 70160.282 | 4.821 | 5.232 | 1.00 | 0.00 H |
| ATOM | 978 | 1HD | ARG A | 70160.658 | 6.931 | 7.352 | 1.00 | 0.00 H |
| ATOM | 979 | 2HD | ARG A | 70160.543 | 5.189 | 7.596 | 1.00 | 0.00 H |
| ATOM | 980 | HE | ARG A | 70162.699 | 5.971 | 5.866 | 1.00 | 0.00 H |
| ATOM | 981 | 1HH1 | ARG A | 70161.731 | 5.474 | 9.181 | 1.00 | 0.00 H |
| ATOM | 982 | 2HH1 | ARG A | 70163.347 | 5.210 | 9.744 | 1.00 | 0.00 H |
| ATOM | 983 | 1HH2 | ARG A | 70164.825 | 5.624 | 6.604 | 1.00 | 0.00 H |
| ATOM | 984 | 2HH2 | ARG A | 70165.104 | 5.296 | 8.282 | 1.00 | 0.00 H |

| ATOM | 985 | N | TYR A | 71157.354 | 7.415 | 3.953 | 1.00 | 0.00 N |
|------|------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 986 | CA | TYR A | 71156.182 | 8.156 | 4.406 | 1.00 | 0.00 C |
| ATOM | 987 | C | TYR A | 71155.796 | 7.749 | 5.824 | 1.00 | 0.00 C |
| ATOM | 988 | О | TYR A | 71155.470 | 8.595 | 6.657 | 1.00 | 0.00 O |
| ATOM | 989 | CB | TYR A | 71155.007 | 7.920 | 3.457 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.195 | 8.551 | 2.094 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.167 | 9.930 | 1.937 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.397 | 7.766 | 0.966 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.337 | 10.510 | 0.693 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.568 | 8.337 | -0.280 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.537 | 9.710 | -0.411 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71155.707 | 10.284 | -1.650 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.249 | 6.486 | 3.661 | 1.00 | 0.00 H |
| ATOM | 998 | HA | TYR A | 71156.432 | 9.207 | 4.401 | 1.00 | 0.00 H |
| ATOM | 999 | 1HB | TYR A | 71154.875 | 6.859 | 3.315 | 1.00 | 0.00 H |
| ATOM | 1000 | 2HB | TYR A | 71154.111 | 8.336 | 3.895 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.010 | 10.555 | 2.804 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.420 | 6.691 | 1.071 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.313 | 11.585 | 0.592 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.725 | 7.710 | -1.145 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71156.632 | 10.235 | -1.902 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72155.835 | 6.447 | 6.092 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.488 | 5.928 | 7.409 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.491 | 4.871 | 7.858 | 1.00 | 0.00 C |
| ATOM | 1009 | О | PHE A | 72157.311 | 4.403 | 7.068 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72154.079 | 5.335 | 7.393 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72153.863 | 4.329 | 6.298 | 1.00 | 0.00 C |

CD1 PHE A 72154.015 6.546 1.00 0.00 C **ATOM** 1012 2.974 CD2 PHE A 5.023 1.00 0.00 C **ATOM** 1013 72153.508 4.738 5.541 1.00 0.00 C **ATOM** 1014 CE1 PHE A 72153.817 2.046 4.015 1.00 0.00 C **ATOM** 1015 CE2 PHE A 72153.309 3.816 **ATOM** 1016 CZ PHE A 72153.463 2.468 4.274 1.00 0.00 C 5.386 1.00 0.00 H **ATOM** 1017 Η PHE A 72156.102 5.823 8.107 1.00 0.00 H **ATOM** 1018 HA PHE A 72155.514 6.751 **ATOM** 1019 1HB PHE A 72153.890 4.844 8.336 1.00 0.00 H 1020 2HB PHE A 6.132 7.260 1.00 0.00 H **ATOM** 72153.361 2.644 7.537 1.00 0.00 H **ATOM** HD1 PHE A 72154.290 1021 **ATOM** 1022 HD2 PHE A 72153.387 5.793 4.820 1.00 0.00 H 72153.939 0.993 5.746 1.00 0.00 H **ATOM** 1023 HE1 PHE A HE2 PHE A 72153.033 4.148 3.024 1.00 0.00 H **ATOM** 1024 HZ PHE A 72153.308 1.744 3.487 1.00 0.00 H **ATOM** 1025 N THR A 73156.422 4.500 9.133 1.00 0.00 N **ATOM** 1026 **ATOM** 1027 CA THR A 73157.326 3.498 9.688 1.00 0.00 C 2.182 **ATOM** 1028 C THR A 73156.594 9.932 1.00 0.00 C THR A 73155.767 2.079 10.838 1.00 0.00 O **ATOM** 1029 Ο **ATOM** 1030 CB THR A 73157.941 4.003 10.993 1.00 0.00 C 11.848 1.00 OG1 THR A 73156.941 4.531 0.00 O **ATOM** 1031 CG2 THR A 73158.983 5.080 10.785 1.00 0.00 C **ATOM** 1032 9.714 1.00 1033 Η THR A 73155.748 4.909 0.00 H **ATOM** HA THR A 73158.114 3.329 8.970 1.00 0.00 H **ATOM** 1034 HBTHR A 73158.417 3.176 11.499 1.00 0.00 H **ATOM** 1035 5.344 11.472 1.00 0.00 H 1036 HG1 THR A 73156.596 **ATOM** 11.742 1.00 0.00 H1037 1HG2 THR A 73159.375 5.392 **ATOM** 10.289 1.00 0.00 H **ATOM** 1038 2HG2 THR A 73158.532 5.927

| ATOM | 1039 | 3HG2 | THR A | 73159.786 | 4.692 | ·10.177 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|---------|------|--------|
| ATOM | 1040 | N | CYS A | 74156.905 | 1.178 | 9.118 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74156.276 | -0.132 | 9.247 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74157.327 | -1.238 | 9.278 | 1.00 | 0.00 C |
| ATOM | 1043 | O | CYS A | 74158.514 | -0.986 | 9.073 | 1.00 | 0.00 O |
| ATOM | 1044 | СВ | CYS A | 74155.305 | -0.369 | 8.090 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYS A | 74153.619 | 0.197 | 8.415 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYS A | 74157.572 | 1.322 | 8.415 | 1.00 | 0.00 H |
| ATOM | 1047 | HA | CYS A | 74155.727 | -0.147 | 10.176 | 1.00 | 0.00 H |
| ATOM | 1048 | IНВ | CYS A | 74155.662 | 0.153 | 7.215 | 1.00 | 0.00 H |
| ATOM | 1049 2 | ΣHB | CYS A | 74155.261 | -1.428 | 7.877 | 1.00 | 0.00 H |
| ATOM | 1050 | HG | CYS A | 74153.098 | 0.048 | 7.623 | 1.00 | 0.00 H |
| ATOM | 1051 | N | ALA A | 75156.880 | -2.462 | 9.536 | 1.00 | 0.00 N |
| ATOM | 1052 | CA | ALA A | 75157.781 | -3.607 | 9.595 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75158.466 | -3.836 | 8.251 | 1.00 | 0.00 C |
| ATOM | 1054 | O | ALA A | 75158.120 | -3.206 | 7.251 | 1.00 | 0.00 O |
| ATOM | 1055 | CB | ALA A | 75157.022 | -4.854 | 10.021 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALA A | 75155.923 | -2.600 | 9.691 | 1.00 | 0.00 H |
| ATOM | 1057 | НА | ALA A | 75158.535 | -3.401 | 10.341 | 1.00 | 0.00 H |
| ATOM | 1058 | lНВ | ALAA | 75156.775 | -5.441 | 9.149 | 1.00 | 0.00 H |
| ATOM | 1059 2 | 2HB | ALA A | 75156.113 | -4.566 | 10.529 | 1.00 | 0.00 H |
| ATOM | 1060 3 | 3HB | ALA A | 75157.636 | -5.441 | 10.687 | 1.00 | 0.00 H |
| ATOM | 1061 | N | LEU A | 76159.440 | -4.741 | 8.235 | 1.00 | 0.00 N |
| ATOM | 1062 | CA | LEU A | 76160.174 | -5.052 | 7.014 | 1.00 | 0.00 C |
| ATOM | 1063 | C | LEU A | 76159.372 | -5.997 | 6.124 | 1.00 | 0.00 C |
| ATOM | 1064 | О | LEU A | 76158.793 | -6.973 | 6.600 | 1.00 | 0.00 O |
| ATOM | 1065 | CB | LEU A | 76161.527 | -5.679 | 7.353 | 1.00 | 0.00 C |

| ATOM | 1066 | CG | LEU A | 76162.600 | -4.692 | 7.818 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|-------|------|--------|
| ATOM | 1067 | CD1 | LEU A | 76163.504 | -5.337 | 8.856 | 1.00 | 0.00 C |
| ATOM | 1068 | CD2 | LEU A | 76163.415 | -4.197 | 6.633 | 1.00 | 0.00 C |
| ATOM | 1069 | H | LEU A | 76159.671 | -5.210 | 9.064 | 1.00 | 0.00 H |
| ATOM | 1070 | НА | LEU A | 76160.339 | -4.129 | 6.482 | 1.00 | 0.00 H |
| ATOM | 1071 | 1HB | LEU A | 76161.376 | -6.410 | 8.135 | 1.00 | 0.00 H |
| ATOM | 1072 | 2HB | LEU A | 76161.895 | -6.189 | 6.475 | 1.00 | 0.00 H |
| ATOM | 1073 | HG | LEU A | 76162.121 | -3.839 | 8.276 | 1.00 | 0.00 H |
| ATOM | 1074 | 1HD1 | LEU A | 76163.112 | -5.145 | 9.844 | 1.00 | 0.00 H |
| ATOM | 1075 | 2HD1 | LEU A | 76164.497 | -4.919 | 8.777 | 1.00 | 0.00 H |
| ATOM | 1076 | 3HD1 | LEU A | 76163.547 | -6.401 | 8.686 | 1.00 | 0.00 H |
| ATOM | 1077 | 1HD2 | LEU A | 76163.394 | -4.936 | 5.846 | 1.00 | 0.00 H |
| ATOM | 1078 | 2HD2 | LEU A | 76164.436 | -4.028 | 6.943 | 1.00 | 0.00 H |
| ATOM | 1079 | 3HD2 | LEU A | 76162.993 | -3.271 | 6.267 | 1.00 | 0.00 H |
| ATOM | 1080 | N | LYS A | 77159.343 | -5.699 | 4.829 | 1.00 | 0.00 N |
| ATOM | 1081 | CA | LYS A | 77158.612 | -6.522 | 3.872 | 1.00 | 0.00 C |
| ATOM | 1082 | C | LYS A | 77157.123 | -6.548 | 4.201 | 1.00 | 0.00 C |
| ATOM | 1083 | О | LYS A | 77156.500 | -7.610 | 4.224 | 1.00 | 0.00 O |
| ATOM | 1084 | СВ | LYS A | 77159.172 | -7.946 | 3.859 | 1.00 | 0.00 C |
| ATOM | 1085 | CG | LYS A | 77160.683 | -8.006 | 3.706 | 1.00 | 0.00 C |
| ATOM | 1086 | CD | LYSA | 77161.119 | -7.581 | 2.314 | 1.00 | 0.00 C |
| ATOM | 1087 | CE | LYS A | 77162.513 | -6.976 | 2.326 | 1.00 | 0.00 C |
| ATOM | 1088 | NZ | LYS A | 77163.560 | -7.995 | 2.614 | 1.00 | 0.00 N |
| ATOM | 1089 | Н | LYSA | 77159.825 | -4.908 | 4.510 | 1.00 | 0.00 H |
| ATOM | 1090 | HA | LYSA | 77158.744 | -6.086 | 2.892 | 1.00 | 0.00 H |
| ATOM | 1091 | 1HB | LYS A | 77158.907 | -8.433 | 4.787 | 1.00 | 0.00 H |
| ATOM | 1092 | 2HB | LYS A | 77158.728 | -8.489 | 3.038 | 1.00 | 0.00 H |

| ATOM | 1093 1HG | LYSA | 77161.135 | -7.344 | 4.431 | 1.00 | 0.00 H |
|------|----------|---------|-----------|---------|-------|------|--------|
| ATOM | 1094 2HG | LYSA | 77161.014 | -9.018 | 3.886 | 1.00 | 0.00 H |
| ATOM | 1095 1HD | LYS A | 77161.120 | -8.447 | 1.668 | 1.00 | 0.00 H |
| ATOM | 1096 2HD | LYSA | 77160.421 | -6.849 | 1.936 | 1.00 | 0.00 H |
| ATOM | 1097 1HE | LYS A | 77162.708 | -6.535 | 1.361 | 1.00 | 0.00 H |
| ATOM | 1098 2HE | LYS A | 77162.552 | -6.209 | 3.086 | 1.00 | 0.00 H |
| ATOM | 1099 1HZ | LYS A | 77163.525 | -8.270 | 3.616 | 1.00 | 0.00 H |
| ATOM | 1100 2HZ | LYS A | 77164.502 | -7.610 | 2.403 | 1.00 | 0.00 H |
| ATOM | 1101 3HZ | LYS A | 77163.404 | -8.841 | 2.028 | 1.00 | 0.00 H |
| ATOM | 1102 N | LYS A | 78156.558 | -5.373 | 4.456 | 1.00 | 0.00 N |
| ATOM | 1103 CA | LYS A | 78155.142 | -5.261 | 4.785 | 1.00 | 0.00 C |
| ATOM | 1104 C | LYS A | 78154.602 | -3.885 | 4.407 | 1.00 | 0.00 C |
| ATOM | 1105 O | LYS A | 78153.781 | -3.312 | 5.123 | 1.00 | 0.00 O |
| ATOM | 1106 CE | LYSA | 78154.921 | -5.517 | 6.278 | 1.00 | 0.00 C |
| ATOM | 1107 CC | S LYS A | 78155.477 | -6.850 | 6.755 | 1.00 | 0.00 C |
| ATOM | 1108 CD | LYS A | 78155.149 | -7.097 | 8.218 | 1.00 | 0.00 C |
| ATOM | 1109 CE | LYSA | 78153.954 | -8.023 | 8.373 | 1.00 | 0.00 C |
| ATOM | 1110 NZ | LYSA | 78153.139 | -7.684 | 9.573 | 1.00 | 0.00 N |
| ATOM | 1111 H | LYS A | 78157.106 | -4.561 | 4.423 | 1.00 | 0.00 H |
| ATOM | 1112 HA | LYS A | 78154.610 | -6.012 | 4.219 | 1.00 | 0.00 H |
| ATOM | 1113 1HB | LYS A | 78155.400 | -4.729 | 6.840 | 1.00 | 0.00 H |
| ATOM | 1114 2HB | LYS A | 78153.861 | - 5.500 | 6.482 | 1.00 | 0.00 H |
| ATOM | 1115 1HG | LYS A | 78155.046 | -7.641 | 6.161 | 1.00 | 0.00 H |
| ATOM | 1116 2HG | LYS A | 78156.550 | -6.845 | 6.631 | 1.00 | 0.00 H |
| ATOM | 1117 1HD | LYS A | 78156.005 | -7.550 | 8.697 | 1.00 | 0.00 H |
| ATOM | 1118 2HD | LYS A | 78154.926 | -6.152 | 8.692 | 1.00 | 0.00 H |
| ATOM | 1119 1HE | LYS A | 78153.332 | -7.938 | 7.493 | 1.00 | 0.00 H |

| ATOM | 1120 2 | HE | LYS A | 78154.309 | -9.038 | 8.464 | 1.00 | 0.00 H |
|--------|--------|-----|-------|-----------|-----------------|--------|------|--------|
| ATOM | 1121 1 | HZ | LYS A | 78152.325 | -8.326 | 9.645 | 1.00 | 0.00 H |
| ATOM | 1122 2 | HZ | LYS A | 78152.792 | -6.707 \ | 9.505 | 1.00 | 0.00 H |
| ATOM | 1123 3 | HZ | LYS A | 78153.716 | -7.775 | 10.433 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.068 | -3.363 | 3.278 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.633 | -2.055 | 2.805 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.555 | -2.020 | 1.282 | 1.00 | 0.00 C |
| ATOM | 1127 | 0 | ALA A | 79155.578 | -1.989 | 0.599 | 1.00 | 0.00 O |
| ATOM | 1128 | СВ | ALÀ A | 79155.571 | -0.971 | 3.312 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79155.721 | -3.869 | 2.751 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.648 | -1.864 | 3.209 | 1.00 | 0.00 H |
| ATOM | 1131 1 | НВ | ALA A | 79156.010 | -1.283 | 4.248 | 1.00 | 0.00 H |
| ATOM 1 | 1132 2 | HB | ALA A | 79155.017 | -0.056 | 3.462 | 1.00 | 0.00 H |
| ATOM | 1133 3 | НВ | ALA A | 79156.353 | -0.802 | 2.586 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.334 | -2.025 | 0.757 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.122 | -1.994 | -0.685 | 1.00 | 0.00 C |
| ATOM | 1136 | C. | LEU A | 80152.248 | -0.809 | -1.081 | 1.00 | 0.00 C |
| ATOM | 1137 | O | LEU A | 80151.047 | -0.791 | -0.810 | 1.00 | 0.00 O |
| ATOM | 1138 | СВ | LEU A | 80152.476 | -3.299 | -1.154 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.145 | -3.358 | -2.647 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.393 | -3.669 | -3.458 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80151.062 | -4.394 | -2.911 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.557 | -2.050 | 1.353 | 1.00 | 0.00 H |
| ATOM | 1143 | НА | LEU A | 80154.086 | -1.889 | -1.160 | 1.00 | 0.00 H |
| ATOM | 1144 1 | НВ | LEU A | 80153.147 | -4.113 | -0.923 | 1.00 | 0.00 H |
| ATOM | 1145 2 | 2HB | LEU A | 80151.559 | -3.442 | -0.600 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.772 | -2.395 | -2.964 | 1.00 | 0.00 H |

| ATOM | 1147 1 | HD1 | LEU A | 80153.335 | -3.169 | -4.413 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1148 2 | 2HD1 | LEU A | 80153.464 | -4.735 | -3.614 | 1.00 | 0.00 H |
| ATOM | 1149 3 | BHD1 | LEU A | 80154.265 | -3.325 | -2.923 | 1.00 | 0.00 H |
| ATOM | 1150 1 | HD2 | LEU A | 80150.263 | -4.270 | -2.196 | 1.00 | 0.00 H |
| ATOM | 1151 2 | 2HD2 | LEU A | 80151.481 | -5.385 | -2.814 | 1.00 | 0.00 H |
| ATOM | 1152 3 | BHD2 | LEU A | 80150.675 | -4.263 | -3.911 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.858 | 0.182 | -1.724 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.135 | 1.371 | -2.158 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.374 | 1.103 | -3.452 | 1.00 | 0.00 C |
| ATOM | 1156 | O | PHE A | 81151.879 | 0.436 | -4.355 | 1.00 | 0.00 O |
| ATOM | 1157 | СВ | PHE A | 81153.104 | 2.538 | -2.355 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.883 | 2.888 | -1.119 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81153.494 | 3.947 | -0.316 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81155.005 | 2.157 | -0.761 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81154.209 | 4.271 | 0.822 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81155.724 | 2.476 | 0.375 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81155.325 | 3.534 | 1.167 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.817 | 0.110 | -1.911 | 1.00 | 0.00 H |
| ATOM | 1165 | НА | PHE A | 81151.428 | 1.630 | -1.385 | 1.00 | 0.00 H |
| ATOM | 1166 1 | НВ | PHE A | 81153.810 | 2.283 | -3.131 | 1.00 | 0.00 H |
| ATOM | 1167 2 | HB | PHE A | 81152.546 | 3.414 | -2.656 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81152.621 | 4.524 | -0.585 | 1.00 | 0.00 H |
| ATOM | 1169 | HD2 | PHE A | 81155.317 | 1.329 | -1.381 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81153.895 | 5.100 | 1.440 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81156.596 | 1.898 | 0.643 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.884 | 3.785 | 2.056 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.155 | 1.628 | -3.535 | 1.00 | 0.00 N |

| ATOM | 1174 | CA | VAL A | 82149.324 | 1.445 | -4.718 | 1.00 | 0.00 C |
|-------------|------|------|-------|-----------|--------|---------|------|--------|
| ATOM | 1175 | C | VALA | 82148.369 | 2.618 | -4.907 | 1.00 | 0.00 C |
| ATOM | 1176 | O | VAL A | 82148.190 | 3.437 | -4.005 | 1.00 | 0.00 O |
| ATOM | 1177 | СВ | VAL A | 82148.507 | 0.142 | -4.635 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VALA | 82149.423 | -1.069 | -4.717 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VAL A | 82147.682 | 0.111 | -3.358 | 1.00 | 0.00 C |
| ATOM | 1180 | Н | VAL A | 82149.807 | 2.151 | -2.782 | 1.00 | 0.00 H |
| ATOM | 1181 | HA | VAL A | 82149.976 | 1.382 | -5.577 | 1.00 | 0.00 H |
| ATOM | 1182 | HB | VAL A | 82147.830 | 0.111 | -5.477 | 1.00 | 0.00 H |
| ATOM | 1183 | 1HG1 | VAL A | 82150.197 | -0.886 | -5.447 | 1.00 | 0.00 H |
| ATOM | 1184 | 2HG1 | VAL A | 82148.848 | -1.936 | -5.010 | 1.00 | 0.00 H |
| ATOM | 1185 | 3HG1 | VAL A | 82149.873 | -1.247 | -3.751 | 1.00 | 0.00 H |
| ATOM | 1186 | 1HG2 | VAL A | 82147.413 | 1.118 | -3.078 | 1.00 | 0.00 H |
| ATOM | 1187 | 2HG2 | VAL A | 82148.261 | -0.341 | -2.566 | 1.00 | 0.00 H |
| ATOM | 1188 | 3HG2 | VAL A | 82146.784 | -0.468 | -3.523 | 1.00 | 0.00 H |
| ATOM | 1189 | N | LYS A | 83147.757 | 2.694 | -6.084 | 1.00 | 0.00 N |
| ATOM | 1190 | CA | LYS A | 83146.820 | 3.768 | -6.391 | 1.00 | 0.00 C |
| ATOM | 1191 | C | LYS A | 83145.576 | 3.672 | -5.515 | 1.00 | 0.00 C |
| ATOM | 1192 | O | LYS A | 83144.875 | 2.659 | -5.521 | 1.00 | 0.00 O |
| ATOM | 1193 | CB | LYS A | 83146.424 | 3.721 | -7.868 | 1.00 | 0.00 C |
| ATOM | 1194 | CG | LYS A | 83147.590 | 3.945 | -8.818 | 1.00 | 0.00 C |
| ATOM | 1195 | CD | LYS A | 83147.222 | 3.577 | -10.246 | 1.00 | 0.00 C |
| ATOM | 1196 | CE | LYS A | 83147.832 | 4.546 | -11.246 | 1.00 | 0.00 C |
| ATOM | 1197 | NZ | LYS A | 83148.273 | 3.859 | -12.490 | 1.00 | 0.00 N |
| ÀTOM | 1198 | Н | LYS A | 83147.941 | 2.011 | -6.763 | 1.00 | 0.00 H |
| ATOM | 1199 | HA | LYS A | 83147.313 | 4.707 | -6.190 | 1.00 | 0.00 H |
| ATOM | 1200 | 1HB | LYS A | 83145.993 | 2.754 | -8.081 | 1.00 | 0.00 H |

| ATOM | 1201 2HB | LYS A | 83145.684 | 4.484 | -8.054 | 1.00 | 0.00 H |
|------|-----------|---------|-----------|---------|--------|------|--------|
| ATOM | 1202 1HG | LYS A | 83147.871 | 4.986 | -8.786 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.421 | 3.334 | -8.500 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83147.587 | 2.583 - | 10.456 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83146.147 | 3.598 - | 10.349 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83147.095 | 5.293 - | 11.500 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83148.686 | 5.025 - | 10.788 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83149.279 | 3.605 - | 12.422 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83148.139 | 4.483 - | 13.310 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83147.717 | 2.991 - | 12.635 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.307 | 4.735 | -4.765 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.147 | 4.776 | -3.883 | 1.00 | 0.00 C |
| ATOM | 1213 C | LEU A | 84142.855 | 4.587 | -4.673 | 1.00 | 0.00 C |
| ATOM | 1214 O | LEU A | 84141.893 | 4.002 | -4.176 | 1.00 | 0.00 O |
| ATOM | 1215 CB | LEU A | 84144.108 | 6.105 | -3.127 | 1.00 | 0.00 C |
| ATOM | 1216 CG | LEU A | 84142.878 | 6.316 | -2.242 | 1.00 | 0.00 C |
| ATOM | 1217 CD | LEU A | 84143.016 | 5.538 | -0.942 | 1.00 | 0.00 C |
| ATOM | 1218 CD2 | 2 LEU A | 84142.672 | 7.795 | -1.961 | 1.00 | 0.00 C |
| ATOM | 1219 H | LEU A | 84145.903 | 5.510 | -4.806 | 1.00 | 0.00 H |
| ATOM | 1220 HA | LEU A | 84144.242 | 3.970 | -3.172 | 1.00 | 0.00 H |
| ATOM | 1221 1HB | LEU A | 84144.989 | 6.165 | -2.504 | 1.00 | 0.00 H |
| ATOM | 1222 2HB | LEU A | 84144.145 | 6.906 | -3.849 | 1.00 | 0.00 H |
| ATOM | 1223 HG | LEU A | 84142.004 | 5.947 | -2.760 | 1.00 | 0.00 H |
| ATOM | 1224 1HD1 | LEU A | 84142.131 | 5.683 | -0.340 | 1.00 | 0.00 H |
| ATOM | 1225 2HD1 | LEU A | 84143.882 | 5.890 | -0.401 | 1.00 | 0.00 H |
| ATOM | 1226 3HD1 | LEU A | 84143.134 | 4.486 | -1.162 | 1.00 | 0.00 H |
| ATOM | 1227 1HD2 | LEU A | 84141.827 | 7.923 | -1.300 | 1.00 | 0.00 H |

| ATOM | 1228 2HD2 LEU A | 84142.485 | 8.316 -2.887 | 1.00 | 0.00 H |
|------|-----------------|-----------|---------------|------|--------|
| ATOM | 1229 3HD2 LEU A | 84143.558 | 8.200 -1.493 | 1.00 | 0.00 H |
| ATOM | 1230 N LYS A | 85142.843 | 5.085 -5.904 | 1.00 | 0.00 N |
| ATOM | 1231 CA LYS A | 85141.670 | 4.971 -6.764 | 1.00 | 0.00 C |
| ATOM | 1232 C LYS A | 85141.371 | 3.510 -7.086 | 1.00 | 0.00 C |
| ATOM | 1233 O LYS A | 85140.226 | 3.147 -7.355 | 1.00 | 0.00 O |
| ATOM | 1234 CB LYS A | 85141.882 | 5.757 -8.059 | 1.00 | 0.00 C |
| ATOM | 1235 CG LYS A | 85143.234 | 5.509 -8.708 | 1.00 | 0.00 C |
| ATOM | 1236 CD LYS A | 85144.209 | 6.639 -8.416 | 1.00 | 0.00 C |
| ATOM | 1237 CE LYS A | 85145.050 | 6.980 -9.635 | 1.00 | 0.00 C |
| ATOM | 1238 NZ LYS A | 85145.823 | 8.237 - 9.443 | 1.00 | 0.00 N |
| ATOM | 1239 H LYSA | 85143.642 | 5.540 -6.244 | 1.00 | 0.00 H |
| ATOM | 1240 HA LYSA | 85140.829 | 5.389 -6.232 | 1.00 | 0.00 H |
| ATOM | 1241 1HB LYS A | 85141.112 | 5.481 -8.764 | 1.00 | 0.00 H |
| ATOM | 1242 2HB LYS A | 85141.798 | 6.812 -7.842 | 1.00 | 0.00 H |
| ATOM | 1243 1HG LYS A | 85143.642 | 4.587 -8.325 | 1.00 | 0.00 H |
| ATOM | 1244 2HG LYS A | 85143.099 | 5.429 -9.776 | 1.00 | 0.00 H |
| ATOM | 1245 1HD LYS A | 85143.653 | 7.515 -8.119 | 1.00 | 0.00 H |
| ATOM | 1246 2HD LYS A | 85144.863 | 6.336 -7.611 | 1.00 | 0.00 H |
| ATOM | 1247 1HE LYS A | 85145.739 | 6.169 -9.820 | 1.00 | 0.00 H |
| ATOM | 1248 2HE LYS A | 85144.396 | 7.096 -10.487 | 1.00 | 0.00 H |
| ATOM | 1249 1HZ LYS A | 85145.341 | 8.853 -8.758 | 1.00 | 0.00 H |
| ATOM | 1250 2HZ LYS A | 85145.911 | 8.745 -10.346 | 1.00 | 0.00 H |
| ATOM | 1251 3HZ LYS A | 85146.777 | 8.020 -9.087 | 1.00 | 0.00 H |
| ATOM | 1252 N SER A | 86142.405 | 2.675 -7.058 | 1.00 | 0.00 N |
| ATOM | 1253 CA SER A | 86142.248 | 1.255 -7.348 | 1.00 | 0.00 C |
| ATOM | 1254 C SER A | 86142.150 | 0.442 -6.061 | 1.00 | 0.00 C |

| ATOM | 1255 | О | SER A | 86142.547 | -0.722 | -6.017 | 1.00 | 0.00 O |
|------|--------|-----|-------|-----------|--------|----------------|-------|--------|
| ATOM | 1256 | СВ | SER A | 86143.421 | 0.752 | -8.193 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.705 | 1.648 | -9.254 | 1.00 | 0.00 O |
| ATOM | 1258 | Н | SER A | 86143.295 | 3.023 | -6.838 | 1.00 | 0.00 H |
| ATOM | 1259 | НА | SER A | 86141.334 | 1.130 | -7.908 | 1.00 | 0.00 H |
| ATOM | 1260 | lНВ | SER A | 86144.298 | 0.663 | -7.569 | 1.00 | 0.00 H |
| ATOM | 1261 2 | ΣНВ | SER A | 86143.176 | -0.214 | -8.608 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86144.344 | 1.247 | -9.848 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYSA | 87141.618 | 1.064 | -5.012 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.467 | 0.398 | -3.724 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87139.994 | 0.260 | -3.353 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYS A | 87139.165 | 1.081 | -3.747 | 1.00 | 0.00 O |
| ATOM | 1267 | CB | CYS A | 87142.207 | 1.175 | -2.634 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYSA | 87143.989 | 0.867 | -2.590 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYS A | 87141.319 | 1.992 | -5.108 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87141.898 | -0.588 | -3.808 | 1.00 | 0.00 H |
| ATOM | 1271 | lНВ | CYS A | 87142.062 | 2.233 | -2.795 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.802 | 0.904 | -1.670 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.418 | 1.539 | -3.125 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.674 | -0.783 | -2.595 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.300 | -1.027 | -2.172 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.226 | -1.247 | -0.662 | 1.00 | 0.00 C |
| ATOM | 1277 | O | ARG A | 88139.134 | -1.828 | -0.067 | 1.00 | 0.00 O |
| ATOM | 1278 | CB | ARG A | 88137.728 | -2.243 | -2.903 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88137.135 | -1.911 | -4.264 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.620 | -1.785 | - 4.199 | .1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.175 | -0.413 | -4.428 | 1.00 | 0.00 N |

| ATOM | 1282 | CZ | ARG A | 88135.192 | 0.183 | -5.618 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1283 | NH1 | ARG A | 88135.631 | -0.468 | -6.688 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88134.768 | 1.433 | -5.740 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.378 | -1.403 | -2.312 | 1.00 | 0.00 H |
| ATOM | 1286 | НА | ARG A | 88137.715 | -0.156 | -2.427 | 1.00 | 0.00 H |
| ATOM | 1287 | 1HB | ARG A | 88138.517 | -2.967 | -3.046 | 1.00 | 0.00 H |
| ATOM | 1288 | 2HB | ARG A | 88136.953 | -2.684 | -2.294 | 1.00 | 0.00 H |
| ATOM | 1289 | 1HG | ARG A | 88137.549 | -0.974 | -4.607 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88137.392 | -2.697 | -4.958 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88135.186 | -2.424 | -4.953 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.285 | -2.103 | -3.222 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88134.846 | 0.092 | -3.655 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88135.952 | -1.412 | -6.603 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88135.640 | -0.016 | -7.580 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88134.436 | 1.929 | -4.938 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88134.780 | 1.881 | -6.634 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.138 | -0.787 | -0.019 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89136.954 | -0.940 | 1.428 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.091 | -2.390 | 1.877 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.444 | -3.284 | 1.330 | 1.00 | 0.00 O |
| ATOM | 1302 | CB | PRO A | 89135.526 | -0.441 | 1.664 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.249 | 0.476 | 0.523 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89136.005 | -0.084 | -0.649 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.650 | -0.326 | 1.981 | 1.00 | 0.00 H |
| ATOM | 1306 | 1HB | PRO A | 89134.846 | -1.280 | 1.672 | 1.00 | 0.00 H |
| ATOM | 1307 | 2HB | PRO A | 89135.476 | 0.079 | 2.609 | 1.00 | 0.00 H |
| ATOM | 1308 | 1HG | PRO A | 89134.189 | 0.491 | 0.314 | 1.00 | 0.00 H |

89135.602 0.758 1.00 0.00 H **ATOM** 1309 2HG PRO A 1.469 1.00 **ATOM** 1310 1HD PRO A 89135.384 -0.771-1.205 0.00 H-1.288 1.00 0.00 H **ATOM** 1311 2HD PRO A 89136.354 0.714 1.00 0.00 N **ATOM** 1312 N **ASP A** 90137.937 -2.618 2.876 **ATOM** 1313 CA **ASP A** 90138.157 -3.961 3.398 1.00 0.00 C 1.00 0.00 C **ATOM** 1314 C ASPA 90137.366 -4.181 4.683 1.00 **ATOM** 1315 O **ASP A** 90137.759 -3.716 5.754 0.00 O **ATOM** 1316 CB ASP A 90139.647 -4.192 3.658 1.00 0.00 C **ATOM** CG ASPA 90140.036 -5.653 3.537 1.00 0.00 C 1317 1.00 **ATOM** 1318 OD1 ASP A 90140.335 -6.275 4.578 0.00 O **ATOM** 1319 OD2 ASP A 90140.041 -6.1742.403 1.00 0.00 O **ATOM** 1320 H **ASP A** 90138.424 -1.866 3.271 1.00 0.00 H**ATOM** 1321 HA ASPA 90137.817 -4.667 2.655 1.00 0.00 H 1.00 0.00 H **ATOM** 1322 1HB **ASP A** 90140.223 -3.6262.941 1.00 0.00 H **ASPA** 90139.889 -3.855 4.654 **ATOM** 1323 2HB **ATOM** 1324 N SER A 91136.249 -4.893 4.571 1.00 0.00 N 1.00 0.00 C **ATOM** 1325 CA SER A 91135.403 -5.173 5.725 6.292 1.00 0.00 C **ATOM** 1326 C SER A 91135.694 -6.560 **ATOM** 1327 O SER A 91134.834 -7.177 6.920 1.00 0.00 O -5.070 1.00 0.00 C 1328 CB SER A 91133.928 5.339 **ATOM** 6.440 1.00 0.00 O 1329 OG SER A 91133.139 -4.656 **ATOM** -5.237 3.691 1.00 0.00 H **ATOM** 1330 H SER A 91135.988 6.482 1.00 0.00 H **ATOM** 1331 HA SER A 91135.620 -4.435 SER A 91133.815 -4.351 4.541 1.00 0.00 H **ATOM** 1332 1HB SER A 91133.577 -6.036 5.005 1.00 0.00 H**ATOM** 1333 2HB 6.584 1.00 0.00 H1334 HG SER A 91132.431 -5.288 **ATOM ATOM** 1335 N ARG A 92136.912 -7.045 6.069 1.00 0.00 N

| ATOM | 1336 | CA | ARG A | 92137.312 | -8.358 | 6.561 | 1.00 | 0.00 C |
|------|------|-------|-------|-------------|---------|--------|------|--------|
| ATOM | 1337 | C | ARG A | 92137.327 | -8.385 | 8.086 | 1.00 | 0.00 C |
| ATOM | 1338 | О | ARG A | 92137.097 | -9.426 | 8.702 | 1.00 | 0.00 O |
| ATOM | 1339 | CB | ARG A | 92138.693 | -8.731 | 6.019 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92138.670 | -9.221 | 4.580 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92137.825 | -10.475 | 4.432 | 1.00 | 0.00 C |
| ATOM | 1342 | NE | ARG A | 92136.492 | -10.179 | 3.911 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92136.232 | -9.956 | 2.624 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92137.209 | -9.994 | 1.726 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92134.992 | -9.695 | 2.235 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92137.557 | -6.509 | 5.564 | 1.00 | 0.00 H |
| ATOM | 1347 | HA | ARG A | 92136.589 | -9.078 | 6.208 | 1.00 | 0.00 H |
| ATOM | 1348 | 1HB | ARG A | 92139.334 | -7.863 | 6.072 | 1.00 | 0.00 H |
| ATOM | 1349 | 2HB | ARG A | 92139.110 | -9.513 | 6.636 | 1.00 | 0.00 H |
| ATOM | 1350 | 1HG | ARG A | 92138.257 | -8.444 | 3.953 | 1.00 | 0.00 H |
| ATOM | 1351 | 2HG | ARG A | 92139.681 | -9.438 | 4.269 | 1.00 | 0.00 H |
| ATOM | 1352 | 1HD | ARG A | 92138.324 | -11.152 | 3.755 | 1.00 | 0.00 H |
| ATOM | 1353 | 2HD | ARG A | 92137.726 | -10.944 | 5.400 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92135.752 | -10.145 | 4.552 | 1.00 | 0.00 H |
| ATOM | 1355 | 1HH1. | ARG A | 92138.147 - | 10.191 | 2.013 | 1.00 | 0.00 H |
| ATOM | 1356 | 2HH1. | ARG A | 92137.007 | -9.826 | 0.761 | 1.00 | 0.00 H |
| ATOM | 1357 | 1HH2 | ARG A | 92134.252 | -9.666 | 2.907 | 1.00 | 0.00 H |
| ATOM | 1358 | 2HH2 | ARG A | 92134.796 | -9.528 | 1.268 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93137.598 | -7.232 | 8.690 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93137.643 | -7.121 | 10.144 | 1.00 | 0.00 C |
| ATOM | 1361 | C | PHE A | 93136.506 | -6.246 | 10.661 | 1.00 | 0.00 C |
| ATOM | 1362 | O | PHE A | 93136.622 | -5.622 | 11.715 | 1.00 | 0.00 O |

| ATOM | 1363 | CB | PHE A | 93138.988 | -6.547 | 10.591 | 1.00 | 0.00 C |
|------|------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 1364 | CG | PHE A | 93140.161 | -7.413 | 10.229 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93140.944 | -7.988 | 11.217 | 1.00 | 0.00 C |
| ATOM | 1366 | CD2 | PHE A | 93140.480 | -7.652 | 8.903 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93142.023 | -8.787 | 10.889 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93141.558 | -8.449 | 8.567 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ | PHE A | 93142.331 | -9.016 | 9.562 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93137.773 | - 6.436 | 8.146 | 1.00 | 0.00 H |
| ATOM | 1371 | НА | PHE A | 93137.532 | -8.114 | 10.555 | 1.00 | 0.00 H |
| ATOM | 1372 | 1HB | PHE A | 93139.132 | -5.582 | 10.125 | 1.00 | 0.00 H |
| ATOM | 1373 | 2HB | PHE A | 93138.981 | -6.425 | 11.664 | 1.00 | 0.00 H |
| ATOM | 1374 | HDI | PHE A | 93140.704 | -7.809 | 12.255 | 1.00 | 0.00 H |
| ATOM | 1375 | HD2 | PHE A | 93139.877 | -7.208 | 8.124 | 1.00 | 0.00 H |
| ATOM | 1376 | HE1 | PHE A | 93142.625 | -9.228 | 11.668 | 1.00 | 0.00 H |
| ATOM | 1377 | HE2 | PHE A | 93141.797 | -8.627 | 7.529 | 1.00 | 0.00 H |
| ATOM | 1378 | HZ | PHE A | 93143.175 | -9.640 | 9.302 | 1.00 | 0.00 H |
| ATOM | 1379 | N | ALA A | 94135.407 | -6.203 | 9.912 | 1.00 | 0.00 N |
| ATOM | 1380 | CA | ALA A | 94134.252 | -5.403 | 10.300 | 1.00 | 0.00 C |
| ATOM | 1381 | C | ALA A | 94133.515 | -6.036 | 11.474 | 1.00 | 0.00 C |
| ATOM | 1382 | O | ALA A | 94133.186 | -7.221 | 11.448 | 1.00 | 0.00 O |
| ATOM | 1383 | CB | ALA A | 94133.311 | -5.227 | 9.116 | 1.00 | 0.00 C |
| ATOM | 1384 | Н | ALA A | 94135.373 | -6.721 | 9.081 | 1.00 | 0.00 H |
| ATOM | 1385 | НА | ALA A | 94134.607 | -4.426 | 10.594 | 1.00 | 0.00 H |
| ATOM | 1386 | 1HB | ALA A | 94133.533 | -4.295 | 8.616 | 1.00 | 0.00 H |
| ATOM | 1387 | 2HB | ALA A | 94132.291 | -5.213 | 9.466 | 1.00 | 0.00 H |
| ATOM | 1388 | 3HB | ALA A | 94133.444 | -6.047 | 8.426 | 1.00 | 0.00 H |
| ATOM | 1389 | N | SER A | 95133.257 | -5.236 | 12.504 | 1.00 | 0.00 N |

| ATOM | 1390 | CA | SER A | 95132.557 | -5.717 | 13.689 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1391 | C | SER A | 95131.078 | -5.939 | 13.396 | 1.00 | 0.00 C |
| ATOM | 1392 | Ο | SER A | 95130.347 | -4.997 | 13.093 | 1.00 | 0.00 O |
| ATOM | 1393 | CB | SER A | 95132.718 | -4.723 | 14.840 | 1.00 | 0.00 C |
| ATOM | 1394 | OG | SER A | 95134.071 | -4.626 | 15.247 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95133.544 | -4.299 | 12.466 | 1.00 | 0.00 H |
| ATOM | 1396 | НА | SER A | 95133.001 | -6.659 | 13.975 | 1.00 | 0.00 H |
| ATOM | 1397 | 1HB | SER A | 95132.379 | -3.748 | 14.522 | 1.00 | 0.00 H |
| ATOM | 1398 | 2HB | SER A | 95132.124 | -5.052 | 15.682 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95134.111 | -4.383 | 16.175 | 1.00 | 0.00 H |
| ATOM | 1400 | N . | LEU A | 96130.643 | -7.192 | 13.488 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96129.250 | -7.537 | 13.233 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96128.828 | -8.744 | 14.064 | 1.00 | 0.00 C |
| ATOM | 1403 | Ο | LEU A | 96128.824 | -9.876 | 13.579 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96129.039 | -7.830 | 11.746 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96128.713 | -6.609 | 10.885 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96129.040 | -6.881 | 9.425 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96127.249 | -6.224 | 11.042 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96131.274 | -7.900 | 13.734 | 1.00 | 0.00 H |
| ATOM | 1409 | HA | LEU A | 96128.642 | -6.691 | 13.513 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96129.940 | -8.286 | 11.359 | 1.00 | 0.00 H |
| ATOM | 1411 | 2HB | LEU A | 96128.229 | -8.537 | 11.650 | 1.00 | 0.00 H |
| ATOM | 1412 | HG | LEU A | 96129.316 | -5.774 | 11.212 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96129.355 | -5.964 | 8.950 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96128.163 | -7.263 | 8.924 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96129.835 | -7.609 | 9.364 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96126.884 | -5.810 | 10.114 | 1.00 | 0.00 H |

1417 2HD2 LEU A 96127.153 -5.488 11.828 1.00 0.00 H**ATOM** 1418 3HD2 LEU A 96126.672 -7.100 11.298 1.00 0.00 H**ATOM** GLN A 97128.471 -8.495 15.320 1.00 0.00 N **ATOM** 1419 N -9.560 16.220 1.00 0.00 C **ATOM** CA GLN A 97128.046 1420 **ATOM** 1421 \mathbf{C} GLN A 97126.659 -9.272 16.790 1.00 0.00 C 16.928 1.00 0.00 O **ATOM** 1422 0 GLN A 97126.264 -8.114 97129.053 -9.725 17.361 1.00 0.00 C **ATOM** 1423 CB GLN A **ATOM** 1424 CG GLN A 97130.174 -10.704 17.045 1.00 0.00 C 97130.874 -11.208 18.292 1.00 0.00 C **ATOM** 1425 CD GLN A 97130.231 -11.632 19.251 1.00 0.00 O **ATOM** 1426 OE1 GLN A **ATOM** 1427 NE2 GLN A 97132.201 -11.162 18.283 1.00 0.00 N GLN A 97128.494 -7.572 15.649 1.00 0.00 H **ATOM** 1428 H 97128.005 -10.478 15.653 1.00 0.00 H **ATOM** 1429 HA GLN A 97129.495 -8.764 17.578 1.00 0.00 H **ATOM** 1430 1HB GLN A 97128.533 -10.079 18.238 1.00 0.00 H **ATOM** 1431 2HB GLN A **ATOM** 1432 1HG GLN A 97129.758 -11.550 16.518 1.00 0.00 H 97130.899 -10.209 **ATOM** 1433 2HG GLN A 16.417 1.00 0.00 H97132.647 -10.812 17.485 1.00 0.00 H**ATOM** 1434 1HE2 GLN A **ATOM** 1435 2HE2 GLN A 97132.681 -11.482 19.076 1.00 0.00 H 98125.898 -10.327 17.129 1.00 0.00 N **ATOM** 1436 N PRO A 1437 CA PRO A 98124.549 -10.181 17.686 1.00 0.00 C **ATOM** PRO A 98124.566 -9.615 19.102 1.00 0.00 C **ATOM** 1438 \mathbf{C} 98125.628 -9.439 19.699 1.00 0.00 O **ATOM** 1439 O PRO A PRO A 98124.009 -11.613 17.690 1.00 0.00 C **ATOM** 1440 CB 0.00 C PRO A 98125.221 -12.475 17.756 1.00 **ATOM** 1441 CG 0.00 C PRO A 98126.294 -11.743 16.998 1.00 1442 CD **ATOM** HA PRO A 98123.928 -9.560 17.059 1.00 0.00 H**ATOM** 1443

| ATOM | 1444 1 | НВ | PRO A | 98123.372 - | 11.758 | 18.549 | 1.00 | 0.00 H | |
|------|--------|-----|---------|--------------|---------|--------|------|--------|--|
| ATOM | 1445 2 | 2HB | PRO A | 98123.448 - | 11.791 | 16.784 | 1.00 | 0.00 H | |
| ATOM | 1446 1 | HG | PRO A | 98125.517 - | -12.613 | 18.785 | 1.00 | 0.00 H | |
| ATOM | 1447 2 | 2HG | PRO A | 98125.019 - | 13.429 | 17.291 | 1.00 | 0.00 H | |
| ATOM | 1448 1 | HD | PRO A | 98127.259 - | 11.917 | 17.448 | 1.00 | 0.00 H | |
| ATOM | 1449 2 | 2HD | PRO A | 98126.297 - | 12.046 | 15.962 | 1.00 | 0.00 H | |
| ATOM | 1450 | N | SER A | 99123.382 | -9.331 | 19.634 | 1.00 | 0.00 N | |
| ATOM | 1451 | CA | SER A | 99123.259 | -8.784 | 20.981 | 1.00 | 0.00 C | |
| ATOM | 1452 | C | SER A | 99122.426 | -9.703 | 21.868 | 1.00 | 0.00 C | |
| ATOM | 1453 | О | SER A | 99121.262 | -9.977 | 21.575 | 1.00 | 0.00 O | |
| ATOM | 1454 | СВ | SER A | 99122.626 | -7.392 | 20.932 | 1.00 | 0.00 C | |
| ATOM | 1455 | OG | SER A | 99123.485 | -6.463 | 20.292 | 1.00 | 0.00 O | |
| ATOM | 1456 | Н | SER A | 99122.570 | -9.493 | 19.109 | 1.00 | 0.00 H | |
| ATOM | 1457 | НА | SER A | 99124.252 | -8.704 | 21.398 | 1.00 | 0.00 H | |
| ATOM | 1458 1 | НВ | SER A | 99121.697 | -7.440 | 20.385 | 1.00 | 0.00 H | |
| ATOM | 1459 2 | 2HB | SER A | 99122.434 | -7.051 | 21.939 | 1.00 | 0.00 H | |
| ATOM | 1460 | HG | SER A | 99123.508 | -5.648 | 20.798 | 1.00 | 0.00 H | |
| ATOM | 1461 | N | GLY A 1 | 00123.030 - | 10.177 | 22.953 | 1.00 | 0.00 N | |
| ATOM | 1462 | CA | GLY A | 100122.328 - | 11.060 | 23.866 | 1.00 | 0.00 C | |
| ATOM | 1463 | C | GLY A 1 | 00123.264 - | 11.750 | 24.840 | 1.00 | 0.00 C | |
| ATOM | 1464 | O | GLY A 1 | 00124.480 - | 11.744 | 24.645 | 1.00 | 0.00 O | |
| ATOM | 1465 | Н | GLY A 1 | 00123.958 | -9.925 | 23.135 | 1.00 | 0.00 H | |
| ATOM | 1466 1 | HA | GLY A 1 | 00121.606 - | 10.483 | 24.424 | 1.00 | 0.00 H | |
| ATOM | 1467 2 | 2HA | GLY A 1 | 00121.806 - | 11.811 | 23.292 | 1.00 | 0.00 H | |
| ATOM | 1468 | N | PRO A | 101122.723 - | 12.361 | 25.909 | 1.00 | 0.00 N | |
| ATOM | 1469 | CA | PRO A | 101123.532 - | 13.058 | 26.914 | 1.00 | 0.00 C | |
| ATOM | 1470 | C | PRO A 1 | 01124.481 - | 14.075 | 26.289 | 1.00 | 0.00 C | |

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| ATOM | 1471 | O | PRO A 101124.058 -15.142 | 25.844 | 1.00 | 0.00 O |
|------|--------|-----|--------------------------|--------|------|--------|
| ATOM | 1472 | СВ | PRO A 101122.490 -13.764 | 27.784 | 1.00 | 0.00 C |
| ATOM | 1473 | CG | PRO A 101121.251 -12.951 | 27.626 | 1.00 | 0.00 C |
| ATOM | 1474 | CD | PRO A 101121.283 -12.419 | 26.220 | 1.00 | 0.00 C |
| ATOM | 1475 | НА | PRO A 101124.098 -12.363 | 27.517 | 1.00 | 0.00 H |
| ATOM | 1476 1 | НВ | PRO A 101122.347 -14.775 | 27.430 | 1.00 | 0.00 H |
| ATOM | 1477 2 | 2HB | PRO A 101122.824 -13.779 | 28.810 | 1.00 | 0.00 H |
| ATOM | 1478 1 | HG | PRO A 101120.382 -13.575 | 27.772 | 1.00 | 0.00 H |
| ATOM | 1479 2 | 2HG | PRO A 101121.254 -12.137 | 28.336 | 1.00 | 0.00 H |
| ATOM | 1480 1 | IHD | PRO A 101120.770 -13.092 | 25.550 | 1.00 | 0.00 H |
| ATOM | 1481 2 | 2HD | PRO A 101120.841 -11.434 | 26.180 | 1.00 | 0.00 H |
| ATOM | 1482 | N | SER A 102125.766 -13.737 | 26.259 | 1.00 | 0.00 N |
| ATOM | 1483 | CA | SER A 102126.776 -14.621 | 25.688 | 1.00 | 0.00 C |
| ATOM | 1484 | C | SER A 102128.162 -14.283 | 26.226 | 1.00 | 0.00 C |
| ATOM | 1485 | O | SER A 102128.405 -13.168 | 26.686 | 1.00 | 0.00 O |
| ATOM | 1486 | СВ | SER A 102126.769 -14.520 | 24.162 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102127.881 -15.196 | 23.599 | 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102126.042 -12.874 | 26.629 | 1.00 | 0.00 H |
| ATOM | 1489 | HA | SER A 102126.528 -15.633 | 25.973 | 1.00 | 0.00 H |
| ATOM | 1490 | IНВ | SER A 102125.863 -14.962 | 23.776 | 1.00 | 0.00 H |
| ATOM | 1491 2 | ΣΗВ | SER A 102126.812 -13.480 | 23.873 | 1.00 | 0.00 H |
| ATOM | 1492 | HG | SER A 102128.175 -14.731 | 22.813 | 1.00 | 0.00 H |
| ATOM | 1493 | N | SER A 103129.067 -15.254 | 26.164 | 1.00 | 0.00 N |
| ATOM | 1494 | CA | SER A 103130.431 -15.060 | 26.645 | 1.00 | 0.00 C |
| ATOM | 1495 | C | SER A 103131.329 -16.216 | 26.219 | 1.00 | 0.00 C |
| ATOM | 1496 | O | SER A 103131.152 -17.349 | 26.666 | 1.00 | 0.00 O |
| ATOM | 1497 | CB | SER A 103130.442 -14.924 | 28.169 | 1.00 | 0.00 C |

SER A 103130.264 -16.183 28.794 1.00 0.00 O **ATOM** 1498 OG 1499 SER A 103128.814 -16.122 25.786 1.00 0.00 H **ATOM** Н **ATOM** 1500 HA SER A 103130.808 -14.146 26.209 1.00 0.00 HSER A 103131.388 -14.510 28.485 1.00 0.00 H **ATOM** 1501 1HB SER A 103129.641 -14.267 28.476 1.00 0.00 H **ATOM** 1502 2HB **ATOM** 1503 HG SER A 103129.437 -16.186 29.280 1.00 0.00 H GLY A 104132.292 -15.922 25.352 0.00 N 1.00 **ATOM** 1504 N 1505 CA GLY A 104133.203 -16.947 24.880 1.00 0.00 C **ATOM** 1.00 · 0.00 C 1506 C GLY A 104132.655 -17.708 23.689 **ATOM** 1.00 0.00 O 1507 O GLY A 104133.079 -17.416 22.551 **ATOM ATOM** 1508 OXT GLY A 104131.800 -18.596 23.893 1.00 0.00 O 0.00 H **ATOM** 1509 H GLY A 104132.385 -15.001 25.030 1.00 0.00 H 1510 1HA GLY A 104134.137 -16.483 24.598 1.00 **ATOM** 1511 2HA GLY A 104133.390 -17.645 25.683 0.00 H**ATOM** 1.00 1512 GLY A 104 TER

ENDMDL

Three-Dimensional Structure Coordinate Table 7

| ATOM 1 | N GLY A | 1128.015 | 1.010 -10.316 | 1.00 | 0.00 N |
|-----------|----------|----------|----------------|------|--------|
| ATOM 2 | CA GLYA | 1127.655 | -0.374 -10.731 | 1.00 | 0.00 C |
| ATOM 3 | C GLY A | 1128.389 | -1.429 -9.927 | 1.00 | 0.00 C |
| ATOM 4 | O GLY A | 1128.645 | -2.528 -10.420 | 1.00 | 0.00 O |
| ATOM 5 1H | I GLY A | 1129.039 | 1.078 -10.148 | 1.00 | 0.00 H |
| ATOM 6 2H | I GLY A | 1127.515 | 1.263 -9.441 | 1.00 | 0.00 H |
| ATOM 7 3H | I GLY A | 1127.751 | 1.686 -11.061 | 1.00 | 0.00 H |
| ATOM 8 1H | IA GLY A | 1126.592 | -0.512 -10.600 | 1.00 | 0.00 H |
| ΔΤΟΜ 9 2E | IA GLYA | 1127 897 | -0.499 -11.776 | 1.00 | 0.00 H |

| ATOM10 | N | SER A | 2128.728 | -1.096 | -8.686 | 1.00 | 0.00 N |
|----------|-----|-------|----------|--------|--------|------|--------|
| ATOM11 | CA | SER A | 2129.437 | -2.024 | -7.813 | 1.00 | 0.00 C |
| ATOM12 | C | SER A | 2128.513 | -2.562 | -6.726 | 1.00 | 0.00 C |
| ATOM13 | О | SER A | 2128.240 | -3.761 | -6.667 | 1.00 | 0.00 O |
| ATOM14 | СВ | SER A | 2130.645 | -1.334 | -7.176 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2131.499 | -0.785 | -8.163 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2128.496 | -0.205 | -8.351 | 1.00 | 0.00 H |
| ATOM17 | HA | SER A | 2129.783 | -2.849 | -8.417 | 1.00 | 0.00 H |
| ATOM18 | IНВ | SER A | 2130.304 | -0.538 | -6.531 | 1.00 | 0.00 H |
| ATOM19 2 | 2HB | SER A | 2131.203 | -2.054 | -6.594 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2132.295 | -0.445 | -7.746 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3128.033 | -1.668 | -5.868 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3127.138 | -2.053 | -4.782 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3125.816 | -1.298 | -4.873 | 1.00 | 0.00 C |
| ATOM24 | O | SER A | 3125.217 | -0.951 | -3.856 | 1.00 | 0.00 O |
| ATOM25 | CB | SER A | 3127.799 | -1.786 | -3.429 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3128.587 | -0.609 | -3.469 | 1.00 | 0.00 O |
| ATOM27 | Н | SER A | 3128.287 | -0.726 | -5.966 | 1.00 | 0.00 H |
| ATOM28 | HA | SER A | 3126.942 | -3.111 | -4.873 | 1.00 | 0.00 H |
| ATOM29 | ΙНВ | SER A | 3127.036 | -1.666 | -2.674 | 1.00 | 0.00 H |
| ATOM30 2 | 2HB | SER A | 3128.434 | -2.620 | -3.170 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3128.100 | 0.088 | -3.915 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4125.367 | -1.048 | -6.099 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4124.119 | -0.335 | -6.299 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4124.265 | 1.160 | -6.100 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4125.326 | 1.638 | -5.697 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4125.887 | -1.348 | -6.873 | 1.00 | 0.00 H |

| ATOM37 | 1HA | GLY A | 4123.769 | -0.521 | -7.304 | 1.00 | 0.00 H |
|--------|-----|-------|----------|--------|--------|------|--------|
| ATOM38 | 2HA | GLY A | 4123.386 | -0.711 | -5.600 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5123.197 | 1.900 | -6.381 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5123.211 | 3.351 | -6.231 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5122.158 | 3.804 | -5.225 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5121.565 | 4.872 | -5.369 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5122.967 | 4.027 | -7.581 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5123.746 | 5.203 | -7.711 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5122.380 | 1.460 | -6.698 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5124.186 | 3.637 | -5.866 | 1.00 | 0.00 H |
| ATOM47 | 1HB | SER A | 5123.231 | 3.346 | -8.376 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5121.923 | 4.291 | -7.665 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5123.666 | 5.731 | -6.914 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6121.929 | 2.982 | -4.205 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6120.947 | 3.298 | -3.175 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6121.634 | 3.702 | -1.874 | 1.00 | 0.00 C |
| ATOM53 | O | SER A | 6122.774 | 3.317 | -1.617 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6120.031 | 2.097 | -2.929 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6119.317 | 1.751 | -4.103 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6122.434 | 2.144 | -4.144 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6120.352 | 4.127 | -3.527 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6120.626 | 1.249 | -2.622 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6119.324 | 2.340 | -2.149 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6118.645 | 1.100 | -3.888 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7120.931 | 4.481 | -1.058 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7121.489 | 4.925 | 0.206 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7122.446 | 6.089 | 0.041 | 1.00 | 0.00 C |

| ATOM64 | Ο | GLY A | 7122.121 | 7.080 | -0.613 | 1.00 | 0.00 O |
|--------|------|-------|----------|--------|--------|------|--------|
| ATOM65 | Н | GLY A | 7120.027 | 4.756 | -1.316 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7120.683 | 5.226 | 0.857 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7122.018 | 4.101 | 0.663 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8123.629 | 5.969 | 0.635 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8124.636 | 7.021 | 0.551 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8125.948 | 6.474 | -0.004 | 1.00 | 0.00 C |
| ATOM71 | Ο | LEU A | 8126.512 | 5.522 | 0.535 | 1.00 | 0.00 O |
| ATOM72 | CB | LEU A | 8124.873 | 7.642 | 1.930 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8123.800 | 8.630 | 2.387 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8123.646 | 8.590 | 3.899 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8124.140 | 10.038 | 1.920 | 1.00 | 0.00 C |
| ATOM76 | H | LEU A | 8123.829 | 5.155 | 1.143 | 1.00 | 0.00 H |
| ATOM77 | НА | LEU A | 8124.266 | 7.782 | -0.119 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8124.930 | 6.843 | 2.656 | 1.00 | 0.00 H |
| ATOM79 | 2HB | LEU A | 8125.821 | 8.158 | 1.911 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8122.852 | 8.351 | 1.948 | 1.00 | 0.00 H |
| ATOM81 | 1HD1 | LEU A | 8122.870 | 7.887 | 4.164 | 1.00 | 0.00 H |
| ATOM82 | 2HD1 | LEU A | 8123.380 | 9.572 | 4.260 | 1.00 | 0.00 H |
| ATOM83 | 3HD1 | LEU A | 8124.579 | 8.282 | 4.347 | 1.00 | 0.00 H |
| ATOM84 | 1HD2 | LEU A | 8124.270 | 10.041 | 0.848 | 1.00 | 0.00 H |
| ATOM85 | 2HD2 | LEU A | 8125.054 | 10.363 | 2.396 | 1.00 | 0.00 H |
| ATOM86 | 3HD2 | LEU A | 8123.337 | 10.709 | 2.187 | 1.00 | 0.00 H |
| ATOM87 | N | ALA A | 9126.427 | 7.081 | -1.085 | 1.00 | 0.00 N |
| ATOM88 | CA | ALA A | 9127.671 | 6.655 | -1.713 | 1.00 | 0.00 C |
| ATOM89 | C | ALA A | 9128.282 | 7.780 | -2.541 | 1.00 | 0.00 C |
| ATOM90 | О | ALAA | 9127.588 | 8.712 | -2.947 | 1.00 | 0.00 O |

| ATOM91 | СВ | ALA | A | 912 | 7.430 | 5.42 | 9 | -2.58 | 30 | 1.00 | 0.00 | C | |
|----------|-----|-----|----|--------------|---------|------|-----|-------|-----|------|------|--------|--|
| ATOM92 | Н | ALA | Α. | 912 | 5.931 | 7.83 | 4 | -1.46 | 8 | 1.00 | 0.00 | Н | |
| ATOM93 | НА | ALA | A | 912 | 8.363 | 6.38 | 31 | -0.92 | 29 | 1.00 | 0.00 | Н | |
| ATOM94 1 | НВ | ALA | Α | 9120 | 6.713 | 4.78 | 2 | -2.09 | 9 | 1.00 | 0.00 | Н | |
| ATOM95 2 | HB | ALA | Α | 9128 | 8.360 | 4.89 | 7 | -2.71 | 7 | 1.00 | 0.00 | Н | |
| ATOM96 3 | НВ | ALA | Α | 912 | 7.047 | 5.73 | 8 | -3.54 | 2 | 1.00 | 0.00 | Н | |
| ATOM97 | N | MET | A | 1012 | 9.585 | 7.68 | 6 | -2.78 | 36 | 1.00 | 0.00 | N | |
| ATOM98 | CA | MET | A | 1013 | 0.290 | 8.69 | 96 | -3.56 | 66 | 1.00 | 0.00 | C | |
| ATOM99 | C | MET | Ά | 1013 | 1.574 | 8.12 | 4 | -4.16 | 53 | 1.00 | 0.00 | C | |
| ATOM | 100 | O | Ml | ETA | 10132. | .645 | 8 | .223 | -3 | 564 | 1.00 | 0.00 O | |
| ATOM | 101 | СВ | M | ET A | 10130 | .617 | 9 | .909 | -2 | .692 | 1.00 | 0.00 C | |
| ATOM | 102 | CG | M | ET A | 10129 | .385 | 10 |).644 | -2 | .188 | 1.00 | 0.00 C | |
| ATOM | 103 | SD | M | E T A | 10129 | .778 | 12 | .268 | -1 | .509 | 1.00 | 0.00 S | |
| ATOM | 104 | CE | M | ET A | 10128 | .986 | 13 | .337 | -2 | .709 | 1.00 | 0.00 C | |
| ATOM | 105 | Н | MI | ET A | 10130. | .084 | 6 | .919 | -2 | .434 | 1.00 | 0.00 H | |
| ATOM | 106 | НА | M | ET A | 10129 | .641 | ç | 800.6 | -4 | .370 | 1.00 | 0.00 H | |
| ATOM | 107 | 1HB | MI | ET A | 10131. | 188 | 9 | .579 | -1. | 838 | 1.00 | 0.00 H | |
| ATOM | 108 | 2HB | MI | ET A | 10131. | 213 | 10 | .602 | -3. | 267 | 1.00 | 0.00 H | |
| ATOM | 109 | 1HG | MI | ET A | 10128. | 697 | 10 | .771 | -3 | 010 | 1.00 | 0.00 H | |
| ATOM | 110 | 2HG | MI | ET A | 10128. | 919 | 10 | .050 | -1. | 416 | 1.00 | 0.00 H | |
| ATOM | 111 | 1HE | ME | TA | 10128. | 189 | 13. | .886 | -2. | 232 | 1.00 | 0.00 H | |
| ATOM | 112 | 2HE | ME | ETA | 10128. | 582 | 12 | .738 | -3. | 512 | 1.00 | 0.00 H | |
| ATOM | 113 | 3HE | ME | ETA | 10129. | 713 | 14 | .030 | -3. | 107 | 1.00 | 0.00 H | |
| ATOM | 114 | N | PR | OA | 11131.4 | 483 | 7. | 516 | -5. | 359 | 1.00 | 0.00 N | |
| ATOM | 115 | CA | PR | OA | 11132. | 643 | 6 | .928 | -6. | 035 | 1.00 | 0.00 C | |
| ATOM | 116 | C | PR | ΟA | 11133.7 | 751 | 7. | 950 | -6. | 283 | 1.00 | 0.00 C | |
| ATOM | 117 | О | PR | OA | 11134.9 | 920 | 7. | 684 | -6. | 004 | 1.00 | 0.00 O | |

| ATOM | 118 | CB | PRO A | 11132.081 | 6.413 | -7.364 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 119 | CG | PRO A | 11130.608 | 6.310 | -7.156 | 1.00 | 0.00 C |
| ATOM | 120 | CD | PRO A | 11130.246 | 7.356 | -6.140 | 1.00 | 0.00 C |
| ATOM | 121 | HA | PRO A | 11133.046 | 6.101 | -5.469 | 1.00 | 0.00 H |
| ATOM | 122 1 | НВ | PRO A | 11132.320 | 7.112 | -8.152 | 1.00 | 0.00 H |
| ATOM | 123 2 | HB | PRO A | 11132.514 | 5.451 | -7.589 | 1.00 | 0.00 H |
| ATOM | 124 1 | HG | PRO A | 11130.095 | 6.502 | -8.085 | 1.00 | 0.00 H |
| ATOM | 125 2 | HG | PRO A | 11130.359 | 5.326 | -6.786 | 1.00 | 0.00 H |
| ATOM | 126 1 | HD | PRO A | 11129.976 | 8.280 | -6.630 | 1.00 | 0.00 H |
| ATOM | 127 2 | HD | PRO A | 11129.437 | 7.010 | -5.514 | 1.00 | 0.00 H |
| ATOM | 128 | N | PRO A | 12133.404 | 9.140 | -6.810 | 1.00 | 0.00 N |
| ATOM | 129 | CA | PRO A | 12134.388 | 10.193 | -7.083 | 1.00 | 0.00 C |
| ATOM | 130 | C | PRO A | 12135.197 | 10.557 | -5.844 | 1.00 | 0.00 C |
| ATOM | 131 | O | PRO A | 12136.300 | 11.094 | -5.944 | 1.00 | 0.00 O |
| ATOM | 132 | СВ | PRO A | 12133.533 | 11.382 | -7.530 | 1.00 | 0.00 C |
| ATOM | 133 | CG | PRO A | 12132.261 | 10.781 | -8.015 | 1.00 | 0.00 C |
| ATOM | 134 | CD | PRO A | 12132.036 | 9.557 | -7.172 | 1.00 | 0.00 C |
| ATOM | 135 | HA | PRO A | 12135.060 | 9.908 | -7.880 | 1.00 | 0.00 H |
| ATOM | 136 1 | НВ | PRO A | 12133.364 | 12.042 | -6.691 | 1.00 | 0.00 H |
| ATOM | 137 2 | 2HB | PRO A | 12134.040 | 11.918 | -8.318 | 1.00 | 0.00 H |
| ATOM | 138 1 | HG | PRO A | 12131.450 | 11.481 | -7.884 | 1.00 | 0.00 H |
| ATOM | 139 2 | 2HG | PRO A | 12132.357 | 10.506 | -9.055 | 1.00 | 0.00 H |
| ATOM | 140 1 | HD | PRO A | 12131.462 | 9.806 | -6.292 | 1.00 | 0.00 H |
| ATOM | 141 2 | 2HD | PRO A | 12131.537 | 8.792 | -7.746 | 1.00 | 0.00 H |
| ATOM | 142 | N | GLY A | 13134.641 | 10.259 | -4.673 | 1.00 | 0.00 N |
| ATOM | 143 | CA | GLY A | 13135.325 | 10.562 | -3.429 | 1.00 | 0.00 C |
| ATOM | 144 | C | GLY A | 13136.013 | 9.350 | -2.835 | 1.00 | 0.00 C |

| ATOM | 145 | O | GLY A | 13135.664 | 8.902 | -1.743 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|--------|---------|------|--------|
| ATOM | 146 | Н | GLY A | 13133.758 | 9.830 | -4.653 | 1.00 | 0.00 H |
| ATOM | 147 | 1HA | GLY A | 13136.063 | 11.328 | -3.615 | 1.00 | 0.00 H |
| ATOM | 148 | 2HA | GLY A | 13134.604 | 10.938 | -2.717 | 1.00 | 0.00 H |
| ATOM | 149 | N | ASN A | 14136.995 | 8.818 | -3.554 | 1.00 | 0.00 N |
| ATOM | 150 | CA | ASN A | 14137.736 | 7.650 | -3.092 | 1.00 | 0.00 C |
| ATOM | 151 | C | ASN A | 14136.803 | 6.459 | -2.890 | 1.00 | 0.00 C |
| ATOM | 152 | O | ASN A | 14136.816 | 5.818 | -1.839 | 1.00 | 0.00 O |
| ATOM | 153 | CB | ASN A | 14138.469 | 7.970 | -1.786 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14139.436 | 9.126 | -1.935 | 1.00 | 0.00 C |
| ATOM | 155 | OD1 | ASN A | 14140.104 | 9.265 | -2.961 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14139.519 | 9.965 | - 0.909 | 1.00 | 0.00 N |
| ATOM | 157 | H | ASN A | 14137.228 | 9.220 | -4.417 | 1.00 | 0.00 H |
| ATOM | 158 | HA | ASN A | 14138.463 | 7.398 | -3.848 | 1.00 | 0.00 H |
| ATOM | 159 | 1HB | ASN A | 14137.743 | 8.227 | -1.028 | 1.00 | 0.00 H |
| ATOM | 160 | 2HB | ASN A | 14139.022 | 7.098 | -1.468 | 1.00 | 0.00 H |
| ATOM | 161 | 1HD2 | ASN A | 14138.958 | 9.793 | -0.124 | 1.00 | 0.00 H |
| ATOM | 162 | 2HD2 | ASN A | 14140.137 | 10.722 | -0.978 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15135.996 | 6.168 | -3.905 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15135.055 | 5.054 | -3.844 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15134.001 | 5.290 | -2.766 | 1.00 | 0.00 C |
| ATOM | 166 | Ο | SER A | 15132.873 | 5.682 | -3.063 | 1.00 | 0.00 O |
| ATOM | 167 | CB | SER A | 15135.798 | 3.742 | -3.575 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15136.062 | 3.049 | -4.783 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15136.034 | 6.716 | -4.718 | 1.00 | 0.00 H |
| ATOM | 170 | HA | SER A | 15134.562 | 4.986 | -4.802 | 1.00 | 0.00 H |
| ATOM | 171 | 1HB | SER A | 15136.736 | 3.957 | -3.085 | 1.00 | 0.00 H |

| ATOM | 172 | 2HB | SER A | 15135.194 | 3.114 | -2.938 | 1.00 | 0.00 H |
|------|-----|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 173 | HG | SER A | 15136.234 | 2.124 | -4.589 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16134.376 | 5.049 | -1.514 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.462 | 5.237 | -0.393 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16134.143 | 5.997 | 0.742 | 1.00 | 0.00 C |
| ATOM | 177 | О | HIS A | 16133.685 | 7.064 | 1.150 | 1.00 | 0.00 O |
| ATOM | 178 | CB | HIS A | 16132.957 | 3.883 | 0.113 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16131.570 | 3.555 | -0.342 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16130.456 | 3.728 | 0.453 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16131.115 | 3.061 | -1.519 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16129.377 | 3.355 | -0.214 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16129.751 | 2.947 | -1.413 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16135.289 | 4.740 | -1.339 | 1.00 | 0.00 H |
| ATOM | 185 | HA | HIS A | 16132.622 | 5.817 | -0.744 | 1.00 | 0.00 H |
| ATOM | 186 | 1HB | HIS A | 16133.616 | 3.105 | -0.245 | 1.00 | 0.00 H |
| ATOM | 187 | 2HB | HIS A | 16132.962 | 3.883 | 1.193 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16130.456 | 4.074 | 1.370 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16131.715 | 2.805 | -2.381 | 1.00 | 0.00 H |
| ATOM | 190 | HE1 | HIS A | 16128.364 | 3.381 | 0.158 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16129.161 | 2.533 | -2.078 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.238 | 5.440 | 1.246 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17135.964 | 6.079 | 2.329 | 1.00 | 0.00 C |
| ATOM | 194 | С | GLY A | 17137.320 | 5.446 | 2.570 | 1.00 | 0.00 C |
| ATOM | 195 | O | GLY A | 17137.588 | 4.929 | 3.654 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.557 | 4.588 | 0.881 | 1.00 | 0.00 H |
| ATOM | 197 | 1HA | GLY A | 17136.104 | 7.122 | 2.087 | 1.00 | 0.00 H |
| ATOM | 198 | 2HA | GLY A | 17135.378 | 6.004 | 3.233 | 1.00 | 0.00 H |

| | | | • | | | | | |
|------|-------|------|-------|-----------|-------|--------|------|--------|
| ATOM | 199 | N | LEU A | 18138.179 | 5.487 | 1.556 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.516 | 4.914 | 1.663 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.514 | 5.950 | 2.171 | 1.00 | 0.00 C |
| ATOM | 202 | O | LEU A | 18140.889 | 6.873 | 1.448 | 1.00 | 0.00 O |
| ATOM | 203 | СВ | LEU A | 18139.972 | 4.374 | 0.306 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18138.938 | 3.521 | -0.431 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18139.197 | 3.545 | -1.929 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18138.957 | 2.092 | 0.092 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.907 | 5.914 | 0.717 | 1.00 | 0.00 H |
| ATOM | 208 | НА | LEU A | 18139.471 | 4.098 | 2.369 | 1.00 | 0.00 H |
| ATOM | 209 | lНВ | LEU A | 18140.231 | 5.213 | -0.323 | 1.00 | 0.00 H |
| ATOM | 210 2 | 2HB | LEU A | 18140.856 | 3.774 | 0.460 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18137.954 | 3.929 | -0.256 | 1.00 | 0.00 H |
| ATOM | 212 | HD1 | LEU A | 18138.664 | 2.732 | -2.399 | 1.00 | 0.00 H |
| ATOM | 213 2 | 2HD1 | LEU A | 18140.255 | 3.436 | -2.114 | 1.00 | 0.00 H |
| ATOM | 214 3 | BHD1 | LEU A | 18138.855 | 4.484 | -2.338 | 1.00 | 0.00 H |
| ATOM | 215 | HD2 | LEU A | 18139.980 | 1.770 | 0.220 | 1.00 | 0.00 H |
| ATOM | 216 2 | 2HD2 | LEU A | 18138.461 | 1.443 | -0.615 | 1.00 | 0.00 H |
| ATOM | 2173 | 3HD2 | LEU A | 18138.445 | 2.050 | 1.041 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19140.937 | 5.792 | 3.420 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.892 | 6.714 | 4.026 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19142.828 | 5.978 | 4.980 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19142.700 | 4.771 | 5.184 | 1.00 | 0.00 O |
| ATOM | 222 | СВ | GLU A | 19141.153 | 7.825 | 4.774 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.096 | 7.312 | 5.737 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19140.078 | 8.078 | 7.045 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19139.086 | 8.792 | 7.302 | 1.00 | 0.00 O |

| ATOM | 226 | OE2 | GLU A | 19141.056 | 7.963 | 7.814 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|-------|-------|------|--------|
| ATOM | 227 | Н | GLU A | 19140.601 | 5.037 | 3.947 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.478 | 7.153 | 3.233 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19141.872 | 8.403 | 5.336 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19140.672 | 8.469 | 4.053 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.127 | 7.406 | 5.270 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19140.294 | 6.271 | 5.948 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.770 | 6.715 | 5.562 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL·A | 20144.726 | 6.133 | 6.495 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.014 | 5.482 | 7.678 | 1.00 | 0.00 C |
| ATOM | 236 | О | VAL A | 20143.052 | 6.032 | 8.215 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20145.712 | 7.194 | 7.023 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20146.786 | 6.547 | 7.885 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VAL A | 20146.337 | 7.962 | 5.868 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.820 | 7.673 | 5.360 | 1.00 | 0.00 H |
| ATOM | 241 | НА | VAL A | 20145.291 | 5.378 | 5.968 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.162 | 7.893 | 7.636 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20146.375 | 6.316 | 8.857 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20147.615 | 7.229 | 7.999 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20147.129 | 5.638 | 7.413 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VALA | 20147.314 | 8.318 | 6.159 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VALA | 20145.708 | 8.802 | 5.613 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20146.431 | 7.310 | 5.012 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.493 | 4.309 | 8.077 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21143.890 | 3.603 | 9.192 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21142.852 | 2.592 | 8.746 | 1.00 | 0.00 C |
| ATOM | 252 | О | GLY A | 21142.800 | 1.477 | 9.261 | 1.00 | 0.00 O |

| ATOM 253 H GLYA 21145.263 3.919 7.611 1.00 0.00 y | |
|--|--|
| ATOM 254 1HA GLYA 21144 666 2 088 0 7 | |
| ATOM 255 2HA GLYA 21143 419 4 221 | |
| ATOM 256 N SER A 22142 024 2 025 | |
| ATOM 257 CA SER A 22140.001 | |
| ATOM 258 C SER A 22141 572 | |
| ATOM 259 O SER A 22142 407 1.041 6.348 1.00 0.00 C | |
| ATOM 260 CB SER 4 22120 000 | |
| ATOM 261 OG SER A 22120 272 | |
| ATOM 262 H SER A 22142.115 | |
| ATOM 263 HA SER A 22142.115 3.887 7.412 1.00 0.00 H | |
| ATOM 264 1HB SER A 22140.312 1.619 8.107 1.00 0.00 H | |
| ATOM 265 2HB SER A 20100 | |
| ATOM 266 HG SER A 2011 | |
| ATOM 267 N LELIA 2014 4.712 7.202 1.00 0.00 H | |
| ATOM 268 CA LELLA 23141.037 -0.171 6.433 1.00 0.00 N | |
| ATOM 269 C LELLA 22141.513 -1.277 5.610 1.00 0.00 C | |
| ATOM 270 O LELIA 22141.115 -1.081 4.150 1.00 0.00 C | |
| ATOM 271 CD - 23140.071 -0.500 3.854 1.00 0.00 O | |
| ATOM 272 CG - 28 ATOM 273 CG - 28 ATOM 274 CG - 28 ATOM 275 CG - 28 ATOM 2 | |
| ATOM 273 CD 2 = 23141.330 -2.942 7.574 1.00 0.00 C | |
| ATOM 274 CD 2 23140.251 -3.798 8.217 1.00 0.00 C | |
| ATOM 275 W - 23142.675 -3.649 7.623 1.00 0.00 C | |
| ATOM 276 H | |
| ATOM 277 HP 23142.590 -1.299 5.677 1.00 0.00 H | |
| ATOM 270 OUR 23139.878 -2.570 6.056 1.00 0.00 H | |
| ATOM 270 VICE ATOM 23141.319 -3.396 5.492 1.00 0.00 H | |
| ATOM 279 HG LEUA 23141.411 -2.026 8.140 1.00 0.00 H | |

| ATOM | 280 | 1HD1 | LEU A | 23140.197 | -3.576 | 9.273 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|---------|--------|------|--------|
| ATOM | 281 | 2HD1 | LEU A | 23140.490 | -4.843 | 8.080 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23139.298 | -3.584 | 7.756 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23143.218 | -3.332 | 8.501 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23143.245 | -3.402 | 6.739 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23142.519 | -4.718 | 7.662 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24141.955 | -1.570 | 3.243 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.691 | -1.451 | 1.815 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.305 | - 2.615 | 1.045 | 1.00 | 0.00 C |
| ATOM | 289 | Ο | ALA A | 24143.292 | -3.209 | 1.480 | 1.00 | 0.00 O |
| ATOM | 290 | СВ | ALA A | 24142.226 | -0.127 | 1.289 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.771 | -2.023 | 3.542 | 1.00 | 0.00 H |
| ATOM | 292 | НА | ALA A | 24140.621 | -1.462 | 1.671 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALA A | 24142.507 | -0.239 | 0.251 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24143.091 | 0.166 | 1.866 | 1.00 | 0.00 H |
| ATOM | 295 | 3HB | ALA A | 24141.461 | 0.630 | 1.375 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.715 | -2.937 | -0.102 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.205 | -4.032 | -0.932 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.605 | -3.530 | -2.316 | 1.00 | 0.00 C |
| ATOM | 299 | O | GLU A | 25142.089 | -2.519 | -2.793 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25141.136 | -5.119 | -1.062 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.708 | -6.516 | -1.245 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.729 | -7.464 | -1.909 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25139.929 | -6.999 | -2.749 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25140.762 | -8.671 | -1.590 | 1.00 | O.00 O |
| ATOM | 305 | Н | GLU A | 25140.932 | -2.428 | -0.396 | 1.00 | 0.00 H |
| ATOM | 306 | НА | GLU A | 25143.075 | -4.452 | -0.449 | 1.00 | 0.00 H |

| ATOM | 307 | 1HB | GLU A | 25140.527 | -5.117 | -0.170 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 308 | 2HB | GLU A | 25140.512 | -4.894 | -1.915 | 1.00 | 0.00 H |
| ATOM | 309 | 1HG | GLU A | 25142.594 | -6.451 | -1.858 | 1.00 | 0.00 H |
| ATOM | 310 | 2HG | GLU A | 25141.970 | -6.913 | -0.275 | 1.00 | 0.00 H |
| ATOM | 311 | N | VALA | 26143.528 | -4.243 | -2.954 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.998 | -3.869 | -4.282 | 1.00 | 0.00 C |
| ATOM | 313 | C | VALA | 26143.826 | -5.020 | -5.268 | 1.00 | 0.00 C |
| ATOM | 314 | О | VAL A | 26144.136 | -6.170 | -4.955 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VAL A | 26145.480 | -3.446 | -4.258 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VAL A | 26145.909 | -2.913 | -5.616 | 1.00 | 0.00 C |
| ATOM | 317 | CG2 | VALA | 26145.722 | -2.410 | -3.170 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.901 | -5.039 | -2.521 | 1.00 | 0.00 H |
| ATOM | 319 | HA | VAL A | 26143.411 | -3.027 | -4.621 | 1.00 | 0.00 H |
| ATOM | 320 | HB | VAL A | 26146.078 | -4.318 | -4.033 | 1.00 | 0.00 H |
| ATOM | 321 | 1HG1 | VAL A | 26145.900 | -1.833 | -5.598 | 1.00 | 0.00 H |
| ATOM | 322 | 2HG1 | VAL A | 26145.225 | -3.266 | -6.374 | 1.00 | 0.00 H |
| ATOM | 323 | 3HG1 | VAL A | 26146.905 | -3.261 | -5.841 | 1.00 | 0.00 H |
| ATOM | 324 | 1HG2 | VAL A | 26146.651 | -2.631 | -2.663 | 1.00 | 0.00 H |
| ATOM | 325 | 2HG2 | VALA | 26144.909 | -2.434 | -2.460 | 1.00 | 0.00 H |
| ATOM | 326 | 3HG2 | VAL A | 26145.781 | -1.428 | -3.616 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYSA | 27143.330 | -4.704 | -6.460 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27143.116 | -5.712 | -7.491 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27144.437 | -6.118 | -8.137 | 1.00 | 0.00 C |
| ATOM | 330 | О | LYS A | 27144.790 | -5.631 | -9.211 | 1.00 | 0.00 O |
| ATOM | 331 | CB | LYS A | 27142.155 | -5.184 | -8.558 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.694 | -5.475 | -8.257 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27139.793 | -4.342 | -8.722 | 1.00 | 0.00 C |

| ATOM | 334 | CE | LYS A | 27138.436 | -4.857 | -9.172 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|----------|--------|------|--------|
| ATOM | 335 | NZ | LYS A | 27137.427 | -4.798 | -8.079 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27143.102 | -3.769 | -6.649 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27142.677 | -6.579 | -7.021 | 1.00 | 0.00 H |
| ATOM | 338 1 | НВ | LYS A | 27142.277 | -4.114 | -8.639 | 1.00 | 0.00 H |
| ATOM | 339 2 | HB | LYS A | 27142.403 | -5.638 | -9.506 | 1.00 | 0.00 H |
| ATOM | 340 1 | HG | LYS A | 27140.405 | -6.382 | -8.767 | 1.00 | 0.00 H |
| ATOM | 341 2 | HG | LYS A | 27140.574 | -5.604 | -7.192 | 1.00 | 0.00 H |
| ATOM | 342 1 | HD | LYS A | 27139.650 | -3.651 | -7.905 | 1.00 | 0.00 H |
| ATOM | 343 2 | HD | LYS A | 27140.268 | -3.833 | -9.549 | 1.00 | 0.00 H |
| ATOM | 344 1 | HE | LYS A | 27138.092 | -4.255 - | 10.000 | 1.00 | 0.00 H |
| ATOM | 345 2 | HE | LYS A | 27138.544 | -5.883 | -9.497 | 1.00 | 0.00 H |
| ATOM | 346 1 | HZ | LYS A | 27136.494 | -4.552 | -8.466 | 1.00 | 0.00 H |
| ATOM | 347 2 | HZ | LYS A | 27137.700 | -4.079 | -7.379 | 1.00 | 0.00 H |
| ATOM | 348 3 | HZ | LYS A | 27137.361 | -5.721 | -7.603 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28145.162 | -7.014 | -7.475 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28146.444 | -7.487 | -7.986 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28146.465 | -9.010 | -8.076 | 1.00 | 0.00 C |
| ATOM | 352 | O | GLU A | 28145.504 | -9.678 | -7.694 | 1.00 | 0.00 O |
| ATOM | 353 | CB | GLU A | 28147.585 | -6.998 | -7.090 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28148.729 | -6.358 | -7.858 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28149.850 | -5.889 | -6.951 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28150.027 | -4.661 | -6.811 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28150.550 | -6.751 | -6.378 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.828 | -7.367 | -6.625 | 1.00 | 0.00 H |
| ATOM | 359 | НА | GLU A | 28146.577 | -7.079 | -8.976 | 1.00 | 0.00 H |
| ATOM | 360 1 | НВ | GLU A | 28147.195 | -6.271 | -6.394 | 1.00 | 0.00 H |

| ATOM | 361 | 2HB | GLU A | 28147.979 | -7.838 | -6.535 | 1.00 | 0.00 H |
|------|-----|------|-------|-------------|-----------|---------|------|--------|
| ATOM | 362 | 1HG | GLU A | 28149.129 | -7.080 | -8.553 | 1.00 | 0.00 H |
| ATOM | 363 | 2HG | GLU A | 28148.348 | -5.507 | -8.404 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29147.568 | -9.551 | -8.582 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29147.716 | -10.996 | -8.721 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29147.613 | -11.688 | -7.363 | 1.00 | 0.00 C |
| ATOM | 367 | Ο | ASN A | 29146.752 | -12.543 | -7.158 | 1.00 | 0.00 O |
| ATOM | 368 | CB | ASN A | 29149.055 | -11.331 | -9.380 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29148.926 | -11.543 | -10.876 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29149.065 | -12.662 - | 11.371 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29148.660 | -10.465 - | 11.605 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29148.301 | -8.967 | -8.868 | 1.00 | 0.00 H |
| ATOM | 373 | НА | ASN A | 29146.915 | -11.351 | -9.353 | 1.00 | 0.00 H |
| ATOM | 374 | 1HB | ASN A | 29149.747 | -10.520 | -9.210 | 1.00 | 0.00 H |
| ATOM | 375 | 2HB | ASN A | 29149.451 | -12.235 | -8.939 | 1.00 | 0.00 H |
| ATOM | 376 | 1HD2 | ASN A | 29148.563 | -9.606 - | 11.144 | 1.00 | 0.00 H |
| ATOM | 377 | 2HD2 | ASN A | 29148.571 - | 10.574 -1 | 2.575 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30148.497 | -11.327 | -6.416 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30148.502 | -11.917 | -5.076 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30147.380 | -11.368 | -4.195 | 1.00 | 0.00 C |
| ATOM | 381 | Ο | PRO A | 30147.416 | -10.208 | -3.786 | 1.00 | 0.00 O |
| ATOM | 382 | CB | PRO A | 30149.865 | -11.505 | -4.521 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30150.175 | -10.219 | -5.206 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30149.559 | -10.314 | -6.578 | 1.00 | 0.00 C |
| ATOM | 385 | НА | PRO A | 30148.437 | -12.993 | -5.117 | 1.00 | 0.00 H |
| ATOM | 386 | 1HB | PRO A | 30149.797 | -11.378 | -3.450 | 1.00 | 0.00 H |
| ATOM | 387 | 2HB | PRO A | 30150.597 | -12.263 | -4.755 | 1.00 | 0.00 H |

0.00 HPRO A 30149.739 -9.397 -4.657 1.00 **ATOM** 388 1HG 0.00 H 389 2HG 30151.244 -10.094 -5.285 1.00 PRO A **ATOM** 1.00 0.00 H 390 1HD PRO A 30149.142 -9.362 -6.870 **ATOM** 1.00 0.00 H 30150.294 -10.640 -7.298 391 2HD PRO A **ATOM** 31146.363 -12.196 -3.889 1.00 0.00 N 392 N PRO A **ATOM** 0.00 C **ATOM** 393 CA PRO A 31145.234 -11.777 -3.052 1.00 0.00 C 31145.642 -11.550 -1.601 1.00 394 C PRO A **ATOM** 31145.519 -12.444 -0.7641.00 0.00 O 395 0 PRO A **ATOM** 0.00 C 1.00 31144.257 -12.951 -3.155 **ATOM** 396 CB PRO A 1.00 0.00 C 31145.111 -14.127 -3.484 **ATOM** 397 CG PRO A 0.00 C **ATOM** 398 CD PRO A 31146.234 -13.598 -4.331 1.00 0.00 H 1.00 **ATOM** 399 HA PRO A 31144.767 -10.882 -3.438 31143.748 -13.083 -2.212 1.00 0.00 H 400 1HB PRO A **ATOM** 0.00 H 31143.537 -12.757 -3.936 1.00 **ATOM** 401 2HB PRO A 0.00 H 31145.499 -14.563 -2.575 1.00 402 1HG PRO A **ATOM** 0.00 H 403 2HG PRO A 31144.536 -14.855 -4.037 1.00 **ATOM** -4.138 0.00 H **ATOM** 404 1HD PRO A 31147.143 -14.148 1.00 0.00 H31145.974 -13.649 -5.3781.00 **ATOM** 405 2HD PRO A 0.00 N 1.00 **ATOM** 406 N PHE A 32146.130 -10.348 -1.310 0.00 C 0.040 1.00 PHE A 32146.557 -10.002 **ATOM** 407 CA 1.00 0.00 C \mathbf{C} PHE A 32145.562 -9.052 0.699 **ATOM** 408 -8.569 0.056 1.00 0.00 O 409 PHE A 32144.630 **ATOM** O 0.009 1.00 0.00 C PHE A 32147.947 -9.364 **ATOM** 410 CB 0.00 C -0.8241.00 CG PHE A 32148.016 -8.116 **ATOM** 411 1.00 0.00 C - 2.056 CD1 PHE A 32148.649 -8.124 412 **ATOM** 1.00 0.00 C CD2 PHE A 32147.447 -6.935 -0.374**ATOM** 413 1.00 0.00 C -6.978 -2.82532148.713 **ATOM** 414 CE1 PHE A

>

| Α' | TOM | 415 | CE2 | PHE A | 32147.508 | -5 785 | -1.139 | 1.00 | 0.00 C |
|----|-----|-------|-----|-------|-------------|----------------|--------|------|--------|
| | TOM | | | • | | | , | | , |
| A | TOM | 416 | CZ | PHE A | 32148.143 | - 5.807 | -2.366 | 1.00 | 0.00 C |
| A | TOM | 417 | Н | PHE A | 32146.203 | -9.678 | -2.022 | 1.00 | 0.00 H |
| A | TOM | 418 | HA | PHE A | 32146.602 | -10.913 | 0.617 | 1.00 | 0.00 H |
| A | TOM | 419 1 | HB | PHE A | 32148.240 | -9.107 | 1.017 | 1.00 | 0.00 H |
| A | TOM | 420 2 | HB | PHE A | 32148.652 - | 10.075 | -0.395 | 1.00 | 0.00 H |
| A | TOM | 421 | HD1 | PHE A | 32149.095 | - 9.039 | -2.416 | 1.00 | 0.00 H |
| A | ТОМ | 422 | HD2 | PHE A | 32146.950 | -6.918 | 0.584 | 1.00 | 0.00 H |
| A | ТОМ | 423 | HE1 | PHE A | 32149.211 | -6.997 | -3.784 | 1.00 | 0.00 H |
| A | ТОМ | 424 | HE2 | PHE A | 32147.060 | -4.872 | -0.778 | 1.00 | 0.00 H |
| A | TOM | 425 | HZ | PHE A | 32148.192 | -4.910 | -2.965 | 1.00 | 0.00 H |
| A | ТОМ | 426 | N | TYR A | 33145.770 | -8.785 | 1.984 | 1.00 | 0.00 N |
| A | ТОМ | 427 | CA | TYR A | 33144.892 | -7.892 | 2.731 | 1.00 | 0.00 C |
| A | TOM | 428 | C | TYR A | 33145.696 | -7.001 | 3.673 | 1.00 | 0.00 C |
| A | ТОМ | 429 | О | TYR A | 33146.335 | -7.487 | 4.607 | 1.00 | 0.00 O |
| A | ТОМ | 430 | СВ | TYR A | 33143.865 | -8.699 | 3.527 | 1.00 | 0.00 C |
| A | TOM | 431 | CG | TYR A | 33142.662 | -9.121 | 2.712 | 1.00 | 0.00 C |
| A | TOM | 432 | CD1 | TYR A | 33141.948 | -8.193 | 1.962 | 1.00 | 0.00 C |
| A | TOM | 433 | CD2 | TYR A | 33142.243 | -10.444 | 2.691 | 1.00 | 0.00 C |
| A | ТОМ | 434 | CE1 | TYR A | 33140.848 | -8.576 | 1.217 | 1.00 | 0.00 C |
| A | TOM | 435 | CE2 | TYR A | 33141.145 | -10.833 | 1.947 | 1.00 | 0.00 C |
| A | TOM | 436 | CZ | TYR A | 33140.452 | -9.896 | 1.212 | 1.00 | 0.00 C |
| A | TOM | 437 | ОН | TYR A | 33139.358 | -10.279 | 0.469 | 1.00 | 0.00 O |
| Α | TOM | 438 | Н | TYR A | 33146.531 | -9.200 | 2.442 | 1.00 | 0.00 H |
| A | TOM | 439 | НА | TYR A | 33144.373 | -7.267 | 2.020 | 1.00 | 0.00 H |
| Α | ТОМ | 440 | IНВ | TYR A | 33144.335 | -9.592 | 3.908 | 1.00 | 0.00 H |
| | TOM | 441 2 | ΣНВ | TYR A | 33143.512 | -8.102 | 4.355 | 1.00 | 0.00 H |
| | | | | | | | | | |

| ATOM | 442 | HD1 | TYR A | 33142.261 | -7.160 | 1.968 | 1.00 | 0.00 H |
|--------|-------|------|-------|-------------|---------------|--------|------|--------|
| ATOM | 443 | HD2 | TYR A | 33142.788 - | 11.177 | 3.268 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33140.306 | -7.840 | 0.641 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.835 - | 11.869 | 1.943 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.593 | -11.028 | -0.083 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.660 | -5.697 | 3.422 | 1.00 | 0.00 N |
| ATOM | 448 | ĊĀ | GLY A | 34146.389 | -4.761 | 4.257 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34145.568 | -3.537 | 4.613 | 1.00 | 0.00 C |
| ATOM | 450 | О | GLY A | 34144.380 | -3.465 | 4.294 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.133 | -5.368 | 2.664 | 1.00 | 0.00 H |
| ATOM | 452 1 | НА | GLY A | 34146.683 | -5.260 | 5.168 | 1.00 | 0.00 H |
| ATOM | 453 2 | 2HA | GLY A | 34147.278 | -4.443 | 3.731 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.200 | -2.573 | 5.275 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VALA | 35145.520 | -1.348 | 5.674 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.266 | -0.117 | 5.168 | 1.00 | 0.00 C |
| ATOM | 457 | O | VAL A | 35147.494 | -0.110 | 5.093 | 1.00 | 0.00 O |
| ATOM | 458 | CB | VALA | 35145.376 | -1.261 | 7.207 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VALA | 35146.742 | -1.264 | 7.877 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35144.581 | -0.024 | 7.601 | 1.00 | 0.00 C |
| ATOM . | 461 | Н | VAL A | 35147.147 | -2.690 | 5.499 | 1.00 | 0.00 H |
| ATOM | 462 | НА | VAL A | 35144.531 | -1.360 | 5.241 | 1.00 | 0.00 H |
| ATOM | 463 | НВ | VAL A | 35144.834 | -2.131 | 7.546 | 1.00 | 0.00 H |
| ATOM | 464 | HG1 | VAL A | 35146.735 | -0.577 | 8.711 | 1.00 | 0.00 H |
| ATOM | 465 2 | 2HG1 | VAL A | 35147.493 | -0.959 | 7.165 | 1.00 | 0.00 H |
| ATOM | 466 3 | 3HG1 | VALA | 35146.965 | -2.258 | 8.232 | 1.00 | 0.00 H |
| ATOM | 467 | HG2 | VALA | 35144.998 | 0.843 | 7.113 | 1.00 | 0.00 H |
| ATOM | 468 2 | 2HG2 | VAL A | 35144.629 | 0.108 | 8.672 | 1.00 | 0.00 H |

| ATOM | 469 | 3HG2 | VAL A | 35143.551 | -0.146 | 7.300 | 1.00 | 0.00 H |
|------|-----|------|-------|-------------|--------|-------|--------|--------|
| ATOM | 470 | N. | ILE A | 36145.515 | 0.923 | 4.822 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.105 | 2.160 | 4.324 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.035 | 2.779 | 5.362 | 1.00 | 0.00 C |
| ATOM | 473 | O | ILE A | 36146.862 | 2.574 | 6.564 | 1.00 | 0.00 O |
| ATOM | 474 | CB | ILE A | 36145.023 | 3.188 | 3.939 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.010 | 2.562 | 2.977 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILEA | 36145.660 | 4.422 | 3.315 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36142.915 | 3.515 | 2.548 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.540 | 0.859 | 4.905 | 1.00 | 0.00 H |
| ATOM | 479 | HA | ILE A | 36146.678 | 1.923 | 3.439 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.512 | 3.494 | 4.840 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.525 | 2.229 | 2.089 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.544 | 1.715 | 3.457 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36146.128 | 5.015 | 4.087 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36144.900 | 5.009 | 2.822 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36146.404 | 4.117 | 2.593 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36142.149 | 3.548 | 3.308 | 1.00 | 0.00 H |
| ATOM | 487 | 2HD1 | ILE A | 36142.486 | 3.173 | 1.617 | 1.00 | 0.00 H |
| ATOM | 488 | 3HD1 | ILE A | 36143.330 | 4.502 | 2.412 | 1.00 | 0.00 H |
| ATOM | 489 | N | ARG A | 37148.020 | 3.537 | 4.891 | 1.00 | 0.00 N |
| ATOM | 490 | CA | ARG A | 37148.977 | 4.184 | 5.780 | 1.00 | 0.00 C |
| ATOM | 491 | C | ARG A | 37149.216 | 5.631 | 5.364 | 1.00 | 0.00 C |
| ATOM | 492 | О | ARG A | 37148.844 | 6.563 | 6.078 | 3 1.00 | 0.00 O |
| ATOM | 493 | CB | ARG A | A 37150.300 | 3.418 | 5.782 | 2 1.00 | 0.00 C |
| ATOM | 494 | CG | ARG A | A 37150.144 | 1.935 | 6.07 | 7 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | A 37150.115 | 1.667 | 7.572 | 2 1.00 | 0.00 C |

| ATOM | 496 | NE | ARG A | 37148.908 | 2.196 | 8.201 | 1.00 | 0.00 N | |
|------|-------|-----|-------|-------------|--------|--------|------|--------|---|
| ATOM | 497 | CZ | ARG A | 37148.788 | 2.420 | 9.508 | 1.00 | 0.00 C | ٠ |
| ATOM | 498 | NH1 | ARG A | 37149.800 | 2.159 | 10.327 | 1.00 | 0.00 N | |
| ATOM | 499 | NH2 | ARG A | 37147.654 | 2.904 | 9.997 | 1.00 | 0.00 N | |
| ATOM | 500 | Н | ARG A | 37148.105 | 3.662 | 3.924 | 1.00 | 0.00 H | |
| ATOM | 501 | НА | ARG A | 37148.563 | 4.173 | 6.778 | 1.00 | 0.00 H | |
| ATOM | 502 1 | НВ | ARG A | 37150.766 | 3.523 | 4.813 | 1.00 | 0.00 H | |
| ATOM | 503 2 | НВ | ARG A | 37150.950 | 3.845 | 6.532 | 1.00 | 0.00 H | |
| ATOM | 504 1 | HG | ARG A | 37149.220 | 1.587 | 5.641 | 1.00 | 0.00 H | |
| ATOM | 505 2 | HG | ARG A | . 37150.976 | 1.402 | 5.640 | 1.00 | 0.00 H | |
| ATOM | 506 1 | HD | ARG A | 37150.154 | 0.600 | 7.734 | 1.00 | 0.00 H | |
| ATOM | 507 2 | HD | ARG A | 37150.979 | 2.130 | 8.025 | 1.00 | 0.00 H | |
| ATOM | 508 | HE | ARG A | 37148.145 | 2.397 | 7.619 | 1.00 | 0.00 H | |
| ATOM | 509 1 | HH1 | ARG A | 37150.657 | 1.793 | 9.966 | 1.00 | 0.00 H | |
| ATOM | 510 2 | HH1 | ARG A | 37149.704 | 2.329 | 11.308 | 1.00 | 0.00 H | |
| ATOM | 511 1 | HH2 | ARG A | 37146.890 | 3.103 | 9.384 | 1.00 | 0.00 H | |
| ATOM | 512 2 | HH2 | ARG A | 37147.565 | 3.072 | 10.979 | 1.00 | 0.00 H | |
| ATOM | 513 | N | TRPA | 38149.841 | 5.814 | 4.206 | 1.00 | 0.00 N | |
| ATOM | 514 | CA | TRPA | 38150.132 | 7.149 | 3.697 | 1.00 | 0.00 C | |
| ATOM | 515 | C | TRP A | 38149.473 | 7.373 | 2.337 | 1.00 | 0.00 C | |
| ATOM | 516 | O | TRPA | 38149.599 | 6.550 | 1.431 | 1.00 | 0.00 O | |
| ATOM | 517 | СВ | TRPA | 38151.647 | 7.361 | 3.589 | 1.00 | 0.00 C | |
| ATOM | 518 | CG | TRPA | 38152.027 | 8.592 | 2.820 | 1.00 | 0.00 C | |
| ATOM | 519 | CD1 | TRP A | 38152.264 | 9.837 | 3.329 | 1.00 | 0.00 C | |
| ATOM | 520 | CD2 | TRPA | 38152.208 | 8.696 | 1.403 | 1.00 | 0.00 C | |
| ATOM | 521 | NE1 | TRPA | 38152.581 | 10.708 | 2.314 | 1.00 | 0.00 N | |
| ATOM | 522 | CE2 | TRPA | 38152.554 | 10.031 | 1.123 | 1.00 | 0.00 C | |

| ATOM | 523 | CE3 | TRPA | 38152.112 | 7.789 | 0.344 | 1.00 | 0.00 C | |
|------|-------|------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 524 | CZ2 | TRPA | 38152.803 | 10.479 | -0.172 | 1.00 | 0.00 C | |
| ATOM | 525 | CZ3 | TRPA | 38152.360 | 8.234 | -0.940 | 1.00 | 0.00 C | |
| ATOM | 526 | CH2 | TRPA | 38152.702 | 9.569 | -1.189 | 1.00 | 0.00 C | |
| ATOM | 527 | Н | TRP A | 38150.114 | 5.032 | 3.682 | 1.00 | 0.00 H | |
| ATOM | 528 | НА | TRPA | 38149.728 | 7.865 | 4.398 | 1.00 | 0.00 H | |
| ATOM | 529 | 1HB | TRP A | 38152.062 | 7.447 | 4.581 | 1.00 | 0.00 H | |
| ATOM | 530 2 | 2HB | TRPA | 38152.086 | 6.508 | 3.092 | 1.00 | 0.00 H | |
| ATOM | 531 | HD1 | TRPA | 38152.207 | 10.086 | 4.378 | 1.00 | 0.00 H | |
| ATOM | 532 | HE1 | TRPA | 38152.794 | 11.659 | 2.426 | 1.00 | 0.00 H | |
| ATOM | 533 | HE3 | TRPA | 38151.849 | 6.756 | 0.517 | 1.00 | 0.00 H | |
| ATOM | 534 | HZ2 | TRPA | 38153.065 | 11.506 | -0.381 | 1.00 | 0.00 H | |
| ATOM | 535 | HZ3 | TRPA | 38152.290 | 7.547 | -1.770 | 1.00 | 0.00 H | |
| ATOM | 536 | HH2 | TRPA | 38152.887 | 9.873 | -2.209 | 1.00 | 0.00 H | |
| ATOM | 537 | N | ILE A | 39148.781 | 8.499 | 2.204 | 1.00 | 0.00 N | |
| ATOM | 538 | CA | ILE A | 39148.111 | 8.845 | 0.957 | 1.00 | 0.00 C | |
| ATOM | 539 | C | ILE A | 39148.616 | 10.185 | 0.433 | 1.00 | 0.00 C | |
| ATOM | 540 | О | ILE A | 39148.281 | 11.239 | 0.974 | 1.00 | 0.00 O | |
| ATOM | 541 | CB | ILE A | 39146.583 | 8.917 | 1.137 | 1.00 | 0.00 C | |
| ATOM | 542 | CG1 | ILE A | 39146.066 | 7.647 | 1.816 | 1.00 | 0.00 C | |
| ATOM | 543 | CG2 | ILE A | 39145.898 | 9.121 | -0.206 | 1.00 | 0.00 C | |
| ATOM | 544 | CD1 | ILE A | 39144.781 | 7.854 | 2.588 | 1.00 | 0.00 C | |
| ATOM | 545 | Н | ILE A | 39148.726 | 9.117 | 2.963 | 1.00 | 0.00 H | |
| ATOM | 546 | HA | ILE A | 39148.335 | 8.077 | 0.231 | 1.00 | 0.00 H | |
| ATOM | 547 | НВ | ILE A | 39146.356 | 9.767 | 1.761 | 1.00 | 0.00 H | |
| ATOM | 548 | 1HG1 | ILE A | 39145.881 | 6.894 | 1.064 | 1.00 | 0.00 H | |
| ATOM | 549 | 2HG1 | ILE A | 39146.814 | 7.285 | 2.506 | 1.00 | 0.00 H | |

| ATOM | 550 | 1HG2 | ILE A | 39146.213 | 8.348 | -0.892 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 551 | 2HG2 | IĻE A | 39146.169 | 10.088 | -0.605 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39144.827 | 9.073 | -0.076 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.535 | 6.952 | 3.127 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39143.983 | 8.092 | 1.900 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39144.908 | 8.668 | 3.286 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.429 | 10.140 | -0.617 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.970 | 11.360 | -1.185 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.570 | 11.152 | -2.561 | 1.00 | 0.00 C |
| ATOM | 559 | O | GLY A | 40150.382 | 10.103 | -3.177 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.667 | 9.272 | -1.006 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40149.179 | 12.091 | -1.257 | 1.00 | 0.00 H |
| ATOM | 562 | 2HA | GLY A | 40150.735 | 11.740 | -0.525 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41151.290 | 12.159 | -3.044 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.919 | 12.094 | -4.355 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41153.396 | 12.478 | -4.267 | 1.00 | 0.00 C |
| ATOM | 566 | Ο | GLN A | 41153.728 | 13.616 | -3.935 | 1.00 | 0.00 O |
| ATOM | 567 | CB | GLN A | 41151.195 | 13.024 | -5.325 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41149.683 | 12.862 | -5.309 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.955 | 14.188 | -5.405 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.905 | 14.953 | -4.443 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41148.387 | 14.464 | -6.571 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41151.398 | 12.969 | -2.505 | 1.00 | 0.00 H |
| ATOM | 573 | HA | GLN A | 41151.839 | 11.080 | -4.713 | 1.00 | 0.00 H |
| ATOM | 574 | 1HB | GLN A | 41151.427 | 14.046 | -5.067 | 1.00 | 0.00 H |
| ATOM | 575 | 2HB | GLN A | 41151.546 | 12.826 | -6.325 | 1.00 | 0.00 H |
| ATOM | 576 | 1HG | GLN A | 41149.390 | 12.247 | -6.145 | 1.00 | 0.00 H |

| ATOM | 577 2HG | GLN A | 41149.396 | 12.376 | -4.388 | 1.00 | 0.00 H |
|------|----------|-------|-----------|--------|--------|------|--------|
| ATOM | 578 1HE2 | GLN A | 41148.468 | 13.805 | -7.292 | 1.00 | 0.00 H |
| ATOM | 579 2HE2 | GLN A | 41147.910 | 15.314 | -6.665 | 1.00 | 0.00 H |
| ATOM | 580 N | PRO A | 42154.309 | 11.532 | -4.559 | 1.00 | 0.00 N |
| ATOM | 581 CA | PRO A | 42155.752 | 11.787 | -4.505 | 1.00 | 0.00 C |
| ATOM | 582 C | PRO A | 42156.172 | 12.938 | -5.414 | 1.00 | 0.00 C |
| ATOM | 583 O | PRO A | 42155.454 | 13.294 | -6.350 | 1.00 | 0.00 O |
| ATOM | 584 CB | PRO A | 42156.371 | 10.471 | -4.989 | 1.00 | 0.00 C |
| ATOM | 585 CG | PRO A | 42155.320 | 9.444 | -4.752 | 1.00 | 0.00 C |
| ATOM | 586 CD | PRO A | 42154.010 | 10.147 | -4.961 | 1.00 | 0.00 C |
| ATOM | 587 HA | PRO A | 42156.079 | 11.991 | -3.496 | 1.00 | 0.00 H |
| ATOM | 588 1HB | PRO A | 42156.616 | 10.552 | -6.039 | 1.00 | 0.00 H |
| ATOM | 589 2HB | PRO A | 42157.265 | 10.260 | -4.420 | 1.00 | 0.00 H |
| ATOM | 590 1HG | PRO A | 42155.429 | 8.634 | -5.458 | 1.00 | 0.00 H |
| ATOM | 591 2HG | PRO A | 42155.389 | 9.074 | -3.739 | 1.00 | 0.00 H |
| ATOM | 592 1HD | PRO A | 42153.719 | 10.100 | -6.000 | 1.00 | 0.00 H |
| ATOM | 593 2HD | PRO A | 42153.244 | 9.717 | -4.331 | 1.00 | 0.00 H |
| ATOM | 594 N | PRO A | 43157.345 | 13.537 | -5.151 | 1.00 | 0.00 N |
| ATOM | 595 CA | PRO A | 43157.858 | 14.653 | -5.950 | 1.00 | 0.00 C |
| ATOM | 596 C | PRO A | 43158.331 | 14.206 | -7.328 | 1.00 | 0.00 C |
| ATOM | 597 O | PRO A | 43159.507 | 13.894 | -7.520 | 1.00 | 0.00 O |
| ATOM | 598 CB | PRO A | 43159.035 | 15.169 | -5.124 | 1.00 | 0.00 C |
| ATOM | 599 CG | PRO A | 43159.493 | 13.989 | -4.340 | 1.00 | 0.00 C |
| ATOM | 600 CD | PRO A | 43158.261 | 13.173 | -4.054 | 1.00 | 0.00 C |
| ATOM | 601 HA | PRO A | 43157.120 | 15.433 | -6.060 | 1.00 | 0.00 H |
| ATOM | 602 1HB | PRO A | 43159.809 | 15.530 | -5.785 | 1.00 | 0.00 H |
| ATOM | 603 2HB | PRO A | 43158.703 | 15.968 | -4.478 | 1.00 | 0.00 H |

| ATOM | 604 1 | HG . | PRO A | 43160.198 | 13.412 | -4.922 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|----------|---------|------|--------|
| ATOM | 605 2 | HG | PRO A | 43159.948 | 14.316 | -3.417 | 1.00 | 0.00 H |
| ATOM | 606 1 | HD | PRO A | 43158.493 | 12.119 | -4.080 | 1.00 | 0.00 H |
| ATOM | 607 2 | HD | PRO A | 43157.843 | 13.445 | -3.096 | 1.00 | 0.00 H |
| ATOM | 608 | N | GLY A | 44157.411 | 14.178 | -8.286 | 1.00 | 0.00 N |
| ATOM | 609 | CA | GLY A | 44157.758 | 13.769 | -9.633 | 1.00 | 0.00 C |
| ATOM | 610 | C | GLY A | 44156.560 | 13.280 - | 10.418 | 1.00 | 0.00 C |
| ATOM | 611 | O | GLY A | 44156.327 | 13.716 - | 11.546 | 1.00 | 0.00 O |
| ATOM | 612 | Н | GLY A | 44156.490 | 14.438 | -8.076 | 1.00 | 0.00 H |
| ATOM | 613 1 | НА | GLY A | 44158.194 | 14.610 - | 10.151 | 1.00 | 0.00 H |
| ATOM | 614 2 | HA | GLY A | 44158.488 | 12.976 | -9.579 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45155.794 | 12.370 | -9.824 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEU A | 45154.613 | 11.822 - | 10.479 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45153.363 | 12.082 | -9.648 | 1.00 | 0.00 C |
| ATOM | 618 | O | LEU A | 45153.203 | 11.525 | -8.562 | 1.00 | 0.00 O |
| ATOM | 619 | CB | LEU A | 45154.783 | 10.318 - | 10.708 | 1.00 | 0.00 C |
| ATOM | 620 | CG · | LEU A | 45155.251 | 9.525 | -9.486 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.856 | 8.060 | -9.614 | 1.00 | 0.00 C |
| ATOM | 622 | CD2 | LEU A | 45156.757 | 9.664 | -9.304 | 1.00 | 0.00 C |
| ATOM | 623 | Н | LEU A | 45156.030 | 12.060 | -8.922 | 1.00 | 0.00 H |
| ATOM | 624 | НА | LEU A | 45154.505 | 12.313 | -11.435 | 1.00 | 0.00 H |
| ATOM | 625 1 | НВ | LEU A | 45153.834 | 9.915 - | 11.032 | 1.00 | 0.00 H |
| ATOM | 626 2 | НВ | LEU A | 45155.504 | 10.175 - | 11.499 | 1.00 | 0.00 H |
| ATOM | 627 | HG | LEU A | 45154.770 | 9.923 | -8.604 | 1.00 | 0.00 H |
| ATOM | 628 1 | HD1 | LEU A | 45154.124 | 7.818 | -8.858 | 1.00 | 0.00 H |
| ATOM | 629 2 | HD1 | LEU A | 45155.729 | 7.438 | -9.480 | 1.00 | 0.00 H |
| ATOM | 630 3 | HD1 | LEU A | 45154.437 | 7.883 - | 10.593 | 1.00 | 0.00 H |

| ATOM | 631 1 | HD2 | LEU A | 45156.974 | 9.910 | -8.275 | 1.00 | 0.00 H | |
|--------------|-------|-----|-------|------------------------|----------|------------------|--------------|------------------|--|
| ATOM | 632 2 | HD2 | LEU A | 45157.127 | 10.451 | -9.947 | 1.00 | 0.00 H | |
| ATOM | 633 3 | HD2 | LEU A | 45157.239 | 8.733 | -9.562 | 1.00 | 0.00 H | |
| ATOM | 634 | N | ASN A | 46152.477 | 12.930 - | -10.162 | 1.00 | 0.00 N | |
| ATOM | 635 | CA | ASN A | 46151.245 | 13.251 | -9.454 | 1.00 | 0.00 C | |
| ATOM | 636 | C | ASN A | 46150.273 | 12.078 | -9.511 | 1.00 | 0.00 C | |
| ATOM | 637 | O | ASN A | 46149.690 | 11.790 | -10.556 | 1.00 | 0.00 O | |
| ATOM | 638 | СВ | ASN A | 46150.597 | 14.498 | -10.061 | 1.00 | 0.00 C | |
| ATOM | 639 | CG | ASN A | 46149.341 | 14.917 | -9.325 | 1.00 | 0.00 C | |
| ATOM | 640 | OD1 | ASN A | 46149.358 | 15.856 | -8.529 | 1.00 | 0.00 O | |
| ATOM | 641 | ND2 | ASN A | 46148.241 | 14.221 | -9.587 | 1.00 | 0.00'N | |
| ATOM | 642 | Н | ASN A | 46152.654 | 13.344 | -11.032 | 1.00 | 0.00 H | |
| ATOM | 643 | НА | ASN A | 46151.494 | 13.450 | -8.423 | 1.00 | 0.00 H | |
| ATOM | 644 1 | НВ | ASN A | 46151.301 | 15.315 - | -10.025 | 1.00 | 0.00 H | |
| ATOM | 645 2 | 2HB | ASN A | 46150.338 | 14.296 - | -11.091 | 1.00 | 0.00 H | |
| ATOM | 646 1 | HD2 | ASN A | 46148.301 | 13.486 - | 10.233 | 1.00 | 0.00 H | |
| ATOM | 647 2 | HD2 | ASN A | 46147.413 | 14.471 | -9.125 | 1.00 | 0.00 H | |
| ATOM | 648 | N | GLU A | 47150.105 | 11.406 | -8.378 | 1.00 | 0.00 N | |
| ATOM | 649 | CA | GLU A | 47149.205 | 10.262 | -8.289 | 1.00 | 0.00 C | |
| ATOM | 650 | C | GLU A | 47148.956 | 9.884 | -6.833 | 1.00 | 0.00 C | |
| ATOM | 651 | O | GLU A | 47149.896 | 9.621 | -6.083 | 1.00 | 0.00 O | |
| ATOM | 652 | CB | GLU A | 47149.782 | 9.066 | -9.049 | 1.00 | 0.00 C | |
| ATOM | 653 | CG | GLU A | 47151.289 | 8.916 | -8.907 | 1.00 | 0.00 C | |
| ATOM | 654 | CD | GLU A | 47151.881 | 7.979 | -9.941 | 1.00 | 0.00 C | |
| ATOM | 655 | OE1 | GLU A | 47152.122 | 8.429 | -11.081 | 1.00 | 0.00 O | |
| | 033 | ODI | | | | | | | |
| ATOM | 656 | | | 47152.104 | 6.795 | -9.612 | 1.00 | 0.00 O | |
| ATOM ATOM | | | GLU A | 47152.104 47150.599 | | -9.612 -7.580 | 1.00 1.00 | 0.00 O 0.00 H | |

| ATOM | 658 | HA | GLU A | 47148.266 | 10.545 | -8.740 | 1.00 | 0.00 H |
|------|-----|------------|-------|-----------|--------|---------|------|--------|
| ATOM | 659 | 1HB | GLU A | 47149.317 | 8.163 | -8.682 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47149.550 | 9.176 | -10.099 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47151.746 | 9.887 | -9.021 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47151.509 | 8.529 | -7.924 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.688 | 9.850 | -6.439 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VAL A | 48147.331 | 9.494 | -5.072 | 1.00 | 0.00 C |
| ATOM | 665 | C | VAL A | 48147.655 | 8.030 | -4.795 | 1.00 | 0.00 C |
| ATOM | 666 | О | VAL A | 48146.912 | 7.133 | -5.191 | 1.00 | 0.00 O |
| ATOM | 667 | СВ | VAL A | 48145.835 | 9.739 | -4.796 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VAL A | 48145.527 | 9.554 | - 3.319 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VALA | 48145.427 | 11.128 | -5.265 | 1.00 | 0.00 C |
| ATOM | 670 | H . | VAL A | 48146.979 | 10.064 | -7.080 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.908 | 10.113 | -4.401 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48145.263 | 9.012 | -5.353 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48145.685 | 8.522 | -3.044 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VAL A | 48144.498 | 9.824 | -3.129 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48146.178 | 10.186 | -2.733 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48145.171 | 11.092 | -6.314 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48146.248 | 11.813 | -5.118 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VAL A | 48144.572 | 11.462 | -4.697 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.771 | 7.795 | -4.114 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49149.196 | 6.439 | -3.787 | 1.00 | 0.00 C |
| ATOM | 681 | C . | LEU A | 49149.018 | 6.158 | -2.301 | 1.00 | 0.00 C |
| ATOM | 682 | Ο | LEU A | 49149.659 | 6.789 | -1.460 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.657 | 6.228 | -4.185 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.989 | 6.568 | -5.640 | 1.00 | 0.00 C |

| ATOM | 685 | CD1 | LEU A | 49152.472 | 6.871 | -5.792 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 686 | CD2 | LEU A | 49150.580 | 5.427 | -6.559 | 1.00 | 0.00 C |
| ATOM | 687 | Н | LEU A | 49149.325 | 8.551 | -3.824 | 1.00 | 0.00 H |
| ATOM | 688 | HA | LEU A | 49148.577 | 5.754 | -4.347 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49151.275 | 6.841 | -3.544 | 1.00 | 0.00 H |
| ATOM | 690 | 2HB | LEU A | 49150.909 | 5.192 | -4.016 | 1.00 | 0.00 H |
| ATOM | 691 | HG | LEU A | 49150.437 | 7.449 | -5.931 | 1.00 | 0.00 H |
| ATOM | 692 | 1HD1 | LEU A | 49152.882 | 7.153 | -4.833 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49152.604 | 7.682 | -6.492 | 1.00 | 0.00 H |
| ATOM | 694 | 3HD1 | LEU A | 49152.984 | 5.993 | -6.157 | 1.00 | 0.00 H |
| ATOM | 695 | 1HD2 | LEU A | 49149.667 | 4.980 | -6.195 | 1.00 | 0.00 H |
| ATOM | 696 | 2HD2 | LEU A | 49151.362 | 4.682 | -6.578 | 1.00 | 0.00 H |
| ATOM | 697 | 3HD2 | LEU A | 49150.421 | 5.808 | -7.556 | 1.00 | 0.00 H |
| ATOM | 698 | N | ALA A | 50148.145 | 5.210 | -1.983 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.887 | 4.849 | -0.596 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALAA | 50148.794 | 3.707 | -0.151 | 1.00 | 0.00 C |
| ATOM | 701 | О | ALA A | 50148.698 | 2.591 | -0.660 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.426 | 4.471 | -0.412 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.665 | 4.741 | -2.698 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50148.091 | 5.718 | 0.013 | 1.00 | 0.00 H |
| ATOM | 705 | 1HB | ALA A | 50146.071 | 4.857 | 0.531 | 1.00 | 0.00 H |
| ATOM | 706 | 2HB | ALA A | 50146.329 | 3.395 | -0.421 | 1.00 | 0.00 H |
| ATOM | 707 | 3НВ | ALA A | 50145.841 | 4.890 | -1.217 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.675 | 3.995 | 0.801 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.587 | 2.981 | 1.299 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51149.892 | 1.946 | 2.160 | 1.00 | 0.00 C |
| ATOM | 711 | О | GLY A | 51149.589 | 2.200 | 3.325 | 1.00 | 0.00 O |

| ATOM | 712 | Η . | GLY A | 51149.707 | 4.902 | 1.170 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 713 | 1HA | GLY A | 51151.047 | 2.483 | 0.458 | 1.00 | 0.00 H |
| ATOM | 714 | 2HA | GLY A | 51151.356 | 3.462 | 1.885 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.638 | 0.775 | 1.585 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52148.973 | -0.303 | 2.309 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52149.989 | -1.169 | 3.048 | 1.00 | 0.00 C |
| ATOM | 718 | Ο | LEU A | 52151.096 | -1.398 | 2.561 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.157 | -1.166 | 1.345 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52146.971 | -0.456 | 0.688 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.473 | -1.249 | -0.511 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEUA | 52145.850 | -0.249 | 1.695 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52149.904 | 0.632 | 0.653 | 1.00 | 0.00 H |
| ATOM | 724 | HA | LEU A | 52148.307 | 0.145 | 3.030 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.816 | -1.520 | 0.565 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52147.780 | -2.018 | 1.889 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.291 | 0.514 | 0.337 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52147.292 | -1.809 | -0.937 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52146.077 | -0.569 | -1.252 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52145.696 | -1.929 | -0.195 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52145.336 | -1.185 | 1.860 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52145.154 | 0.482 | 1.314 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52146.266 | 0.102 | 2.628 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53149.603 | -1.646 | 4.227 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.479 | -2.487 | 5.035 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53149.945 | -3.914 | 5.110 | 1.00 | 0.00 C |
| ATOM | 737 | О | GLU A | 53148.905 | -4.167 | 5.719 | 1.00 | 0.00 O |
| ATOM | 738 | СВ | GLU A | 53150.619 | -1.908 | 6.444 | 1.00 | 0.00 C |

| ATOM | 739 | CG | GLU A | 53151.548 | -2.709 | 7.342 | 1.00 | 0.00 C |
|--------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 740 | CD | GLU A | 53151.003 | -2.872 | 8.747 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53150.405 | -3.929 | 9.034 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53151.176 | -1.940 | 9.563 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53148.708 | -1.428 | 4.562 | 1.00 | 0.00 H |
| ATOM | 744 | НА | GLU A | 53151.451 | -2.503 | 4.564 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.004 | -0.902 | 6.370 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53149.644 | -1.877 | 6.907 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53151.686 | -3.690 | 6.911 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53152.500 | -2.203 | 7.396 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54150.663 | -4.842 | 4.488 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.262 | -6.244 | 4.484 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54150.392 | -6.851 | 5.878 | 1.00 | 0.00 C |
| ATOM | 752 | O | LEU A | 54151.214 | -6.411 | 6.682 | 1.00 | 0.00 O |
| ATOM | 753 | CB | LEU A | 54151.110 | -7.037 | 3.488 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.206 | -6.425 | 2.090 | 1.00 | 0.00 C |
| ATOM . | 755 | CD1 | LEU A | 54152.397 | -6.999 | 1.338 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEU A | 54149.919 | -6.664 | 1.315 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.483 | -4.580 | 4.020 | 1.00 | 0.00 H |
| ATOM | 758 | НА | LEU A | 54149.227 | -6.292 | 4.180 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.108 | -7.127 | 3.890 | 1.00 | 0.00 H |
| ATOM | 760 | 2HB | LEU A | 54150.687 | -8.026 | 3.396 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.352 | -5.358 | 2.180 | 1.00 | 0.00 H |
| ATOM | 762 | 1HD1 | LEU A | 54152.143 | -7.976 | 0.952 | 1.00 | 0.00 H |
| ATOM | 763 | 2HD1 | LEU A | 54153.239 | -7.086 | 2.009 | 1.00 | 0.00 H |
| ATOM | 764 | 3HD1 | LEU A | 54152.656 | -6.345 | 0.519 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54149.250 | -5.828 | 1.463 | 1.00 | 0.00 H |

| ATOM | 766 2 | HD2 | LEU A | 54149.448 | -7.569 | 1.667 | 1.00 | 0.00 H |
|------|-------|-----|--------------------|-------------|---------|--------|------|--------|
| ATOM | 767 3 | HD2 | LEU A | 54150.145 | -6.761 | 0.263 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55149.577 | -7.864 | 6.156 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55149.603 | -8.531 | 7.451 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55150.652 | -9.638 | 7.472 | 1.00 | 0.00 C |
| ATOM | 771 | O | GLU A | 55151.247 | -9.925 | 8.511 | 1.00 | 0.00 O |
| ATOM | 772 | CB | GLU A | 55148.225 | -9.112 | 7.777 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55147.239 | -8.081 | 8.300 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55147.170 | -8.058 | 9.815 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55146.195 | -8.603 | 10.374 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55148.091 | -7.495 | 10.444 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU ⁻ A | 55148.945 | -8.169 | 5.473 | 1.00 | 0.00 H |
| ATOM | 778 | HA | GLU A | 55149.859 | -7.795 | 8.199 | 1.00 | 0.00 H |
| ATOM | 779 1 | HB | GLU A | 55147.812 | -9.551 | 6.880 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55148.339 | -9.882 | 8.525 | 1.00 | 0.00 H |
| ATOM | 781 | HG | GLU A | 55147.543 | -7.103 | 7.955 | 1.00 | 0.00 H |
| ATOM | 782 2 | 2HG | GLU A | 55146.258 | -8.311 | 7.913 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56150.874 - | 10.258 | 6.317 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASPA | 56151.851 | -11.333 | 6.202 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASPA | 56153.173 - | 10.811 | 5.649 | 1.00 | 0.00 C |
| ATOM | 786 | O | ASPA | 56153.208 - | -10.169 | 4.599 | 1.00 | O.00 O |
| ATOM | 787 | CB | ASPA | 56151.313 | -12.446 | 5.301 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56150.352 | -13.365 | 6.029 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASPA | 56149.236 - | 13.588 | 5.512 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56150.715 - | 13.864 | 7.114 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.368 | -9.984 | 5.523 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.022 | -11.733 | 7.190 | 1.00 | 0.00 H |

| ATOM | 793 1HB | ASPA | 56150.793 -12.004 | 4.464 | 1.00 | 0.00 H | |
|------|---------|---------|-------------------|----------|------|--------|---|
| ATOM | 794 2HB | ASPA | 56152.140 -13.036 | 4.934 | 1.00 | 0.00 H | |
| ATOM | 795 N | GLU A | 57154.259 -11.088 | 6.363 | 1.00 | 0.00 N | |
| ATOM | 796 CA | GLU A | 57155.584 -10.645 | 5.943 | 1.00 | 0.00 C | |
| ATOM | 797 C | GLU A | 57156.033 -11.387 | 4.689 | 1.00 | 0.00 C | |
| ATOM | 798 O | GLU A | 57156.555 -12.499 | 4.766 | 1.00 | 0.00 O | |
| ATOM | 799 CB | GLU A | 57156.597 -10.862 | 7.068 | 1.00 | 0.00 C | |
| ATOM | 800 CG | GLU A | 57156.634 - 9.72 | 8 8.079 | 1.00 | 0.00 C | |
| ATOM | 801 CD | GLU A | 57157.934 -9.68 | 86 8.859 | 1.00 | 0.00 C | |
| ATOM | 802 OE | 1 GLU A | 57158.886 -9.025 | 8.391 | 1.00 | 0.00 O | |
| ATOM | 803 OE | 2 GLU A | 57158.001 -10.312 | 9.938 | 1.00 | 0.00 O | |
| ATOM | 804 H | GLU A | 57154.167 -11.603 | 7.192 | 1.00 | 0.00 H | |
| ATOM | 805 HA | GLU A | 57155.525 -9.59 | 0 5.722 | 1.00 | 0.00 H | |
| ATOM | 806 1HB | GLU A | 57156.348 -11.774 | 7.591 | 1.00 | 0.00 H | |
| ATOM | 807 2HB | GLU A | 57157.582 -10.963 | 6.636 | 1.00 | 0.00 H | |
| ATOM | 808 1HG | GLU A | 57156.517 -8.79 | 2 7.557 | 1.00 | 0.00 H | |
| ATOM | 809 2HG | GLU A | 57155.819 -9.85 | 6 8.776 | 1.00 | 0.00 H | |
| ATOM | 810 N | CYS A | 58155.825 -10.764 | 3.533 | 1.00 | 0.00 N | |
| ATOM | 811 CA | CYS A | 58156.210 -11.364 | 2.261 | 1.00 | 0.00 C | |
| ATOM | 812 C | CYS A | 58157.455 -10.689 | 1.695 | 1.00 | 0.00 C | |
| ATOM | 813 O | CYS A | 58157.512 -9.46 | 5 1.580 | 1.00 | 0.00 O | |
| ATOM | 814 CB | CYSA | 58155.060 -11.263 | 3 1.258 | 1.00 | 0.00 C | |
| ATOM | 815 SG | CYSA | 58155.200 -12.400 | -0.142 | 1.00 | 0.00 S | |
| ATOM | 816 H | CYS A | 58155.405 -9.87 | 9 3.536 | 1.00 | 0.00 H | |
| ATOM | 817 HA | CYS A | 58156.429 -12.40 | 6 2.440 | 1.00 | 0.00 H | ٠ |
| ATOM | 818 1HB | CYS A | 58154.131 -11.480 | 1.763 | 1.00 | 0.00 H | |
| ATOM | 819 2HB | CYS A | 58155.023 -10.257 | 0.864 | 1.00 | 0.00 H | |

| ATOM | 820 | HG | CYS A | 58155.346 | -13.282 | 0.206 | 1.00 | 0.00 H |
|------|--------------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 821 | N | ALA A | 59158.450 | -11.497 | 1.343 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALAA | 59159.695 | -10.978 | 0.787 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59159.453 | -10.283 | -0.548 | 1.00 | 0.00 C |
| ATOM | 824 | О | ALAA | 59158.956 | -10.893 | -1.495 | 1.00 | 0.00 O |
| ATOM | 825 | СВ | ALAA | 59160.709 | -12.100 | 0.625 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALA A | 59158.345 | -12.464 | 1.458 | 1.00 | 0.00 H |
| ATOM | 827 | НА | ALA A | 59160.097 | -10.259 | 1.487 | 1.00 | 0.00 H |
| ATOM | 828 | IНВ | ALA A | 59161.226 | -12.256 | 1.561 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59161.421 | -11.833 | -0.141 | 1.00 | 0.00 H |
| ATOM | 830 3 | ЗНВ | ALA A | 59160.197 | -13.008 | 0.341 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60159.808 | -9.005 | -0.618 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60159.622 | -8.249 | -1.842 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60159.105 | -6.847 | -1.587 | 1.00 | 0.00 C |
| ATOM | 834 | O | GLY A | 60159.364 | -5.931 | -2.367 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60160.200 | -8.570 | 0.169 | 1.00 | 0.00 H |
| ATOM | 836 | 1HA | GLY A | 60160.568 | -8.184 | -2.359 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60158.916 | -8.772 | -2.471 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61158.372 | -6.679 | -0.491 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61157.818 | -5.378 | -0.135 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61158.817 | -4.564 | 0.680 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61159.828 | -5.091 | 1.147 | 1.00 | 0.00 O |
| ATOM | 842 | CB | CYS A | 61156.519 | -5.553 | 0.656 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYSA | 61155.273 | -6.557 | -0.185 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61158.200 | -7.447 | 0.092 | 1.00 | 0.00 H |
| ATOM | 845 | HA | CYS A | 61157.602 | -4.848 | -1.050 | 1.00 | 0.00 H |
| ATOM | 846 | 1HB | CYS A | 61156.742 | -6.029 | 1.598 | 1.00 | 0.00 H |

| ATOM | 847 | 2HB | CYS A | 61156.087 | -4.581 | 0.843 | 1.00 | 0.00 H |
|-------------------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 848 | HG | CYS A | 61154.755 | -7.009 | 0.485 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.529 | -3.278 | 0.848 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.402 | -2.391 | 1.608 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62158.917 | -2.249 | 3.047 | 1.00 | 0.00 C |
| ATOM | 852 | О | THR A | 62157.942 | -2.885 | 3.448 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62159.471 | -1.016 | 0.942 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.253 | -0.718 | 0.283 | 1.00 | 0.00 O |
| ATOM . | 855 | CG2 | THR A | 62160.584 | -0.898 | -0.076 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62157.709 | -2.916 | 0.453 | 1.00 | 0.00 H |
| ATOM [*] | 857 | НА | THR A | 62160.390 | -2.827 | 1.616 | 1.00 | 0.00 H |
| ATOM | 858 | HB | THR A | 62159.637 | -0.267 | 1.703 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62158.243 | 0.209 | 0.033 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62161.538 | -0.993 | 0.421 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62160.526 | 0.064 | -0.563 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62160.483 | -1.681 | -0.812 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASP A | 63159.602 | -1.412 | 3.818 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASP A | 63159.240 | -1.185 | 5.212 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.612 | 0.192 | 5.394 | 1.00 | 0.00 C |
| ATOM | 866 | O | ASP A | 63158.751 | 0.814 | 6.448 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASPA | 63160.473 | -1.319 | 6.108 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.586 | -0.372 | 5.706 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63162.107 | -0.513 | 4.580 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63161.935 | 0.512 | 6.517 | 1.00 | 0.00 O |
| ATOM | 871 | Н | ASP A | 63160.370 | -0.933 | 3.440 | 1.00 | 0.00 H |
| ATOM | 872 | НА | ASPA | 63158.518 | -1.938 | 5.493 | 1.00 | 0.00 H |
| ATOM | 873 | 1HB | ASP A | 63160.193 | -1.104 | 7.129 | 1.00 | 0.00 H |

| ATOM | 874 2 | 2HB | ASP A | 63160.846 | -2.331 | 6.048 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 875 | N | GLY A | 64157.919 | 0.662 | 4.363 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.278 | 1.963 | 4.429 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64158.053 | 3.031 | 3.681 | 1.00 | 0.00 C |
| ATOM | 878 | O | GLY A | 64158.129 | 4.177 | 4.125 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64157.841 | 0.122 | 3.548 | 1.00 | 0.00 H |
| ATOM | 880 1 | ΙHΑ | GLY A | 64156.289 | 1.887 | 4.004 | 1.00 | 0.00 H |
| ATOM | 881 2 | 2HA | GLY A | 64157.192 | 2.256 | 5.466 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.628 | 2.654 | 2.544 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.401 | 3.587 | 1.733 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65159.066 | 3.428 | 0.253 | 1.00 | 0.00 C |
| ATOM | 885 | O | THR A | 65159.267 | 2.360 | -0.328 | 1.00 | 0.00 O |
| ATOM | 886 | CB | THR A | 65160.898 | 3.371 | 1.955 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.198 | 1.990 | 2.046 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.419 | 4.037 | 3.210 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.532 | 1.726 | 2.243 | 1.00 | 0.00 H |
| ATOM | 890 | НА | THR A | 65159.141 | 4.589 | 2.042 | 1.00 | 0.00 H |
| ATOM | 891 | НВ | THR A | 65161.439 | 3.780 | 1.113 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65160.877 | 1.539 | 1.261 | 1.00 | 0.00 H |
| ATOM | 893 | HG2 | THR A | 65161.665 | 5.067 | 2.995 | 1.00 | 0.00 H |
| ATOM | 894 2 | 2HG2 | THR A | 65162.303 | 3.520 | 3.551 | 1.00 | 0.00 H |
| ATOM | 895 3 | 3HG2 | THR A | 65160.661 | 4.001 | 3.978 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.556 | 4.496 | -0.352 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.193 | 4.473 | -1.764 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.281 | 5.122 | -2.615 | 1.00 | 0.00 C |
| ATOM | 899 | O | PHE A | 66159.440 | 6.343 | -2.613 | 1.00 | 0.00 O |
| ATOM | 900 | СВ | PHE A | 66156.862 | 5.195 | -1.982 | 1.00 | 0.00 C |

| ATOM | 901 | CG · | PHE A | 66156.296 | 5.008 | -3.360 | 1.00 | 0.00 C |
|------|-------|----------|-------|-----------|-------|---------|------|--------|
| ATOM | 902 | CD1 | PHE A | 66155.867 | 3.760 | -3.784 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66156.194 | 6.080 | -4.233 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.346 | 3.585 | -5.052 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.674 | 5.910 | -5.502 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66155.249 | 4.662 | -5.912 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.419 | 5.317 | 0.164 | 1.00 | 0.00 H |
| ATOM | 908 | НА | PHE A | 66158.086 | 3.442 | -2.063 | 1.00 | 0.00 H |
| ATOM | 909 1 | НВ | PHE A | 66156.138 | 4.821 | -1.272 | 1.00 | 0.00 H |
| ATOM | 910 2 | 2HB | PHE A | 66157.004 | 6.254 | -1.820 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66155.942 | 2.918 | -3.112 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.525 | 7.056 | -3.913 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66155.016 | 2.608 | -5.371 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.599 | 6.754 | -6.172 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.843 | 4.527 | -6.904 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67160.027 | 4.296 | -3.341 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67161.100 | 4.789 | -4.198 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67162.157 | 5.521 | -3.378 | 1.00 | 0.00 C |
| ATOM | 919 | 0 | ARG A | 67162.675 | 6.557 | -3.798 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67160.534 | 5.719 | -5.274 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67159.459 | 5.073 | -6.133 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67159.356 | 5.744 | -7.493 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67159.127 | 4.777 | -8.564 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67159.155 | 5.084 | - 9.859 | 1.00 | 0.00 C |
| ATOM | 925 | NHI | ARG A | 67159.400 | 6.331 | -10.247 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67158.938 | 4.145 | -10.769 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.851 | 3.333 | -3.302 | 1.00 | 0.00 H |

| ATOM | 928 | HA | ARG A | 67161.559 | 3.937 | -4.677 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|----------|--------|------|--------|
| ATOM | 929 1 | НВ | ARG A | 67160.107 | 6.587 | -4.794 | 1.00 | 0.00 H |
| ATOM | 930 2 | HB | ARG A | 67161.340 | 6.035 | -5.920 | 1.00 | 0.00 H |
| ATOM | 931 1 | HG | ARG A | 67159.705 | 4.031 | -6.275 | 1.00 | 0.00 H |
| ATOM | 932 2 | HG | ARG A | 67158.509 | 5.156 | -5.626 | 1.00 | 0.00 H |
| ATOM | 933 1 | HD | ARG A | 67158.534 | 6.444 | -7.473 | 1.00 | 0.00 H |
| ATOM | 934 2 | HD | ARG A | 67160.275 | 6.275 | -7.690 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67158.944 | 3.850 | -8.305 | 1.00 | 0.00 H |
| ATOM | 936 1 | HH1 | ARG A | 67159.565 | 7.044 | -9.566 | 1.00 | 0.00 H |
| ATOM | 937 2 | HH1 | ARG A | 67159.421 | 6.555 -1 | 11.221 | 1.00 | 0.00 H |
| ATOM | 938 1 | HH2 | ARG A | 67158.753 | 3.205 -1 | 0.481 | 1.00 | 0.00 H |
| ATOM | 939 2 | HH2 | ARG A | 67158.958 | 4.375 -1 | 11.741 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.473 | 4.977 | -2.208 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.468 | 5.592 | -1.349 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.935 | 6.814 | -0.627 | 1.00 | 0.00 C |
| ATOM | 943 | О | GLY A | 68163.691 | 7.728 | -0.297 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68162.027 | 4.152 | -1.926 | 1.00 | 0.00 H |
| ATOM | 945 1 | HA | GLY A | 68163.792 | 4.868 | -0.617 | 1.00 | 0.00 H |
| ATOM | 946 2 | НА | GLY A | 68164.315 | 5.885 | -1.950 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.629 | 6.830 | -0.382 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.994 | 7.950 | 0.305 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69160.067 | 7.454 | 1.411 | 1.00 | 0.00 C |
| ATOM | 950 | О | THR A | 69158.900 | 7.147 | 1.164 | 1.00 | 0.00 O |
| ATOM | 951 | СВ | THR A | 69160.209 | 8.807 | -0.689 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.975 | 9.048 | -1.855 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69159.796 | 10.148 | -0.125 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69161.078 | 6.073 | -0.669 | 1.00 | 0.00 H |

| ATOM | 955 H | HA THR A | 69161.774 | 8.551 | 0.749 | 1.00 | 0.00 H | |
|------|--------|-----------|-----------|--------|--------|------|--------|--|
| ATOM | 956 H | IB THR A | 69159.312 | 8.277 | -0.974 | 1.00 | 0.00 H | |
| ATOM | 957 H | IG1 THR A | 69160.699 | 8.445 | -2.550 | 1.00 | 0.00 H | |
| ATOM | 958 1H | G2 THR A | 69160.366 | 10.356 | 0.768 | 1.00 | 0.00 H | |
| ATOM | 959 2H | G2 THR A | 69158.743 | 10.129 | 0.117 | 1.00 | 0.00 H | |
| ATOM | 960 3H | G2 THR A | 69159.982 | 10.920 | -0.858 | 1.00 | 0.00 H | |
| ATOM | 961 N | N ARGA | 70160.593 | 7.377 | 2.629 | 1.00 | 0.00 N | |
| ATOM | 962 C | CA ARGA | 70159.811 | 6.918 | 3.771 | 1.00 | 0.00 C | |
| ATOM | 963 C | C ARG A | 70158.618 | 7.835 | 4.018 | 1.00 | 0.00 C | |
| ATOM | 964 C | O ARG A | 70158.749 | 9.059 | 4.005 | 1.00 | 0.00 O | |
| ATOM | 965 C | CB ARGA | 70160.689 | 6.855 | 5.023 | 1.00 | 0.00 C | |
| ATOM | 966 C | CG ARGA | 70159.948 | 6.370 | 6.260 | 1.00 | 0.00 C | |
| ATOM | 967 C | CD ARGA | 70160.069 | 7.358 | 7.410 | 1.00 | 0.00 C | |
| ATOM | 968 N | NE ARGA | 70160.228 | 6.685 | 8.697 | 1.00 | 0.00 N | |
| ATOM | 969 C | CZ ARGA | 70161.380 | 6.178 | 9.131 | 1.00 | 0.00 C | |
| ATOM | 970 N | NH1 ARG A | 70162.475 | 6.264 | 8.385 | 1.00 | 0.00 N | |
| ATOM | 971 N | NH2 ARG A | 70161.437 | 5.582 | 10.315 | 1.00 | 0.00 N | |
| ATOM | 972 I | H ARGA | 70161.529 | 7.635 | 2.762 | 1.00 | 0.00 H | |
| ATOM | 973 I | HA ARGA | 70159.448 | 5.926 | 3.546 | 1.00 | 0.00 H | |
| ATOM | 974 1H | IB ARGA | 70161.513 | 6.181 | 4.838 | 1.00 | 0.00 H | |
| ATOM | 975 2H | IB ARGA | 70161.079 | 7.841 | 5.225 | 1.00 | 0.00 H | |
| ATOM | 976 1H | IG ARGA | 70158.904 | 6.245 | 6.016 | 1.00 | 0.00 H | |
| ATOM | 977 2H | IG ARGA | 70160.363 | 5.421 | 6.567 | 1.00 | 0.00 H | |
| ATOM | 978 1H | ID ARGA | 70160.928 | 7.989 | 7.237 | 1.00 | 0.00 H | |
| ATOM | 979 2H | ID ARGA | 70159.177 | 7.966 | 7.440 | 1.00 | 0.00 H | |
| ATOM | 980 I | HE ARG | 70159.436 | 6.606 | 9.267 | 1.00 | 0.00 H | |
| ATOM | 981 1H | HI ARG A | 70162.438 | 6.711 | 7.492 | 1.00 | 0.00 H | |

| ATOM | 982 2 | HH1 | ARG A | 70163.337 | 5.881 | 8.717 | 1.00 | 0.00 H |
|--------|--------|----------|-------|-----------|--------|--------|------|--------|
| ATOM | 983 1 | HH2 | ARG A | 70160.615 | 5.515 | 10.880 | 1.00 | 0.00 H |
| ATOM | 984 2 | 2HH2 . | ARG A | 70162.303 | 5.202 | 10.641 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.454 | 7.233 | 4.243 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71156.236 | 7.995 | 4.494 | 1.00 | 0.00 C |
| ATOM | 987 | 1 C | TYR A | 71155.691 | 7.705 | 5.889 | 1.00 | 0.00 C |
| ATOM | 988 | O | TYR A | 71155.213 | 8.606 | 6.578 | 1.00 | 0.00 O |
| ATOM | 989 | СВ | TYR A | 71155.177 | 7.661 | 3.442 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.365 | 8.402 | 2.137 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.369 | 7.722 | 0.925 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.540 | 9.780 | 2.117 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.542 | 8.396 | -0.270 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.713 | 10.460 | 0.926 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.713 | 9.764 | -0.263 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71155.885 | 10.437 | -1.451 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.415 | 6.255 | 4.240 | 1.00 | 0.00 H |
| ATOM | 998 | НА | TYR A | 71156.481 | 9.044 | 4.426 | 1.00 | 0.00 H |
| ATOM | 999 | lНВ | TYR A | 71155.209 | 6.604 | 3.230 | 1.00 | 0.00 H |
| ATOM | 1000 2 | 2HB | TYR A | 71154.202 | 7.916 | 3.831 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.235 | 6.651 | 0.924 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.541 | 10.323 | 3.050 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.541 | 7.849 | -1.202 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.847 | 11.532 | 0.931 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71155.181 | 10.199 | -2.060 | 1.00 | 0.00 H |
| ATOM . | 1006 | N | PHE A | 72155.770 | 6.445 | 6.299 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.285 | 6.036 | 7.613 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.210 | 4.994 | 8.234 | 1.00 | 0.00 C |

| ATOM | 1009 | O | PHE A | 72157.229 | 4.626 | 7.649 | 1.00 | 0.00 O | |
|------|------|-----|-------|-----------|-------|--------|------|--------|--|
| ATOM | 1010 | СВ | PHE A | 72153.866 | 5.476 | 7.505 | 1.00 | 0.00 C | |
| ATOM | 1011 | CG | PHE A | 72153.694 | 4.488 | 6.386 | 1.00 | 0.00 C | |
| ATOM | 1012 | CD1 | PHE A | 72153.520 | 4.923 | 5.082 | 1.00 | 0.00 C | |
| ATOM | 1013 | CD2 | PHE A | 72153.705 | 3.126 | 6.639 | 1.00 | 0.00 C | |
| ATOM | 1014 | CE1 | PHE A | 72153.360 | 4.017 | 4.050 | 1.00 | 0.00 C | |
| ATOM | 1015 | CE2 | PHE A | 72153.546 | 2.215 | 5.612 | 1.00 | 0.00 C | |
| ATOM | 1016 | CZ | PHE A | 72153.374 | 2.662 | 4.316 | 1.00 | 0.00 C | |
| ATOM | 1017 | Н | PHE A | 72156.163 | 5.772 | 5.705 | 1.00 | 0.00 H | |
| ATOM | 1018 | НА | PHE A | 72155.270 | 6.910 | 8.247 | 1.00 | 0.00 H | |
| ATOM | 1019 | 1HB | PHE A | 72153.612 | 4.977 | 8.429 | 1.00 | 0.00 H | |
| ATOM | 1020 | 2HB | PHE A | 72153.176 | 6.290 | 7.341 | 1.00 | 0.00 H | |
| ATOM | 1021 | HDI | PHE A | 72153.509 | 5.983 | 4.874 | 1.00 | 0.00 H | |
| ATOM | 1022 | HD2 | PHE A | 72153.839 | 2.776 | 7.652 | 1.00 | 0.00 H | |
| ATOM | 1023 | HE1 | PHE A | 72153.225 | 4.369 | 3.039 | 1.00 | 0.00 H | |
| ATOM | 1024 | HE2 | PHE A | 72153.557 | 1.156 | 5.822 | 1.00 | 0.00 H | |
| ATOM | 1025 | HZ | PHE A | 72153.250 | 1.952 | 3.511 | 1.00 | 0.00 H | |
| ATOM | 1026 | N | THR A | 73155.849 | 4.521 | 9.422 | 1.00 | 0.00 N | |
| ATOM | 1027 | CA | THR A | 73156.646 | 3.521 | 10.122 | 1.00 | 0.00 C | |
| ATOM | 1028 | C | THR A | 73155.862 | 2.224 | 10.297 | 1.00 | 0.00 C | |
| ATOM | 1029 | О | THR A | 73154.872 | 2.180 | 11.028 | 1.00 | 0.00 O | |
| ATOM | 1030 | CB | THR A | 73157.085 | 4.053 | 11.487 | 1.00 | 0.00 C | |
| ATOM | 1031 | OG1 | THR A | 73157.756 | 3.047 | 12.225 | 1.00 | 0.00 O | |
| ATOM | 1032 | CG2 | THR A | 73155.934 | 4.552 | 12.333 | 1.00 | 0.00 C | |
| ATOM | 1033 | Н | THR A | 73155.026 | 4.853 | 9.839 | 1.00 | 0.00 H | |
| ATOM | 1034 | HA | THR A | 73157.523 | 3.320 | 9.526 | 1.00 | 0.00 H | |
| ATOM | 1035 | HB | THR A | 73157.767 | 4.877 | 11.339 | 1.00 | 0.00 H | |

| ATOM | 1036 | HG1 | THR A | 73158.668 | 3.311 | 12.370 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|---------------------|
| ATOM | 1037 1 | HG2 | THR A | 73156.046 | 5.613 | 12.504 | 1.00 | 0.00 H |
| ATOM | 1038 2 | HG2 | THR A | 73155.932 | 4.033 | 13.281 | 1.00 | 0.00 H |
| ATOM | 1039 3 | HG2 | THR A | 73155.002 | 4.368 | 11.819 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYS A | 74156.311 | 1.172 | 9.622 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74155.651 | -0.126 | 9.704 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74156.672 | -1.259 | 9.654 | 1.00 | 0.00 C |
| ATOM | 1043 | O | CYS A | 74157.867 | -1.025 | 9.475 | 1.00 | 0.00 O |
| ATOM | 1044 | СВ | CYS A | 74154.644 | -0.282 | 8.562 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYS A | 74152.993 | 0.348 | 8.944 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYS A | 74157.105 | 1.270 | 9.056 | 1.00 | 0.00 H |
| ATOM | 1047 | НА | CYS A | 74155.125 | -0.172 | 10.644 | 1.00 | 0.00 H |
| ATOM | 1048 1 | НВ | CYS A | 74155.007 | 0.252 | 7.697 | 1.00 | 0.00 H |
| ATOM | 1049 2 | 2HB | CYS A | 74154.548 | -1.330 | 8.318 | 1.00 | 0.00 H |
| ATOM | 1050 | HG | CYS A | 74153.037 | 0.799 | 9.791 | 1.00 | 0.00 H |
| ATOM | 1051 | N | ALA A | 75156.192 | -2.488 | 9.816 | 1.00 | 0.00 N |
| ATOM | 1052 | CA | ALA A | 75157.063 | -3.657 | 9.791 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75157.708 | -3.832 | 8.420 | 1.00 | 0.00 _. C |
| ATOM | 1054 | O | ALAA | 75157.169 | -3.385 | 7.408 | 1.00 | 0.00 O |
| ATOM | 1055 | СВ | ALA A | 75156.281 | -4.906 | 10.171 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALAA | 75155.231 | -2.611 | 9.956 | 1.00 | 0.00 H |
| ATOM | 1057 | HA | ALA A | 75157.840 | -3.510 | 10.527 | 1.00 | 0.00 H |
| ATOM | 1058 | lНВ | ALA A | 75155.259 | -4.806 | 9.836 | 1.00 | 0.00 H |
| ATOM | 1059 2 | 2HB | ALA A | 75156.298 | -5.028 | 11.244 | 1.00 | 0.00 H |
| ATOM | 1060 | знв | ALA A | 75156.730 | -5.769 | 9.703 | 1.00 | 0.00 H |
| ATOM | 1061 | N | LEU A | 76158.864 | -4.486 | 8.395 | 1.00 | 0.00 N |
| ATOM | 1062 | CA | LEU A | 76159.583 | -4.720 | 7.148 | 1.00 | 0.00 C |

| ATOM | 1063 | C | LEU A | 76158.884 | -5.784 | 6.309 | 1.00 | 0.00 C | |
|------|------|------|-------|-----------|--------|-------|------|--------|--|
| ATOM | 1064 | О | LEU A | 76158.277 | -6.711 | 6.844 | 1.00 | 0.00 O | |
| ATOM | 1065 | CB | LEU A | 76161.023 | -5.147 | 7.437 | 1.00 | 0.00 C | |
| ATOM | 1066 | CG | LEU A | 76161.915 | -4.055 | 8.031 | 1.00 | 0.00 C | |
| ATOM | 1067 | CD1 | LEU A | 76161.985 | -4.187 | 9.545 | 1.00 | 0.00 C | |
| ATOM | 1068 | CD2 | LEU A | 76163.309 | -4.116 | 7.425 | 1.00 | 0.00 C | |
| ATOM | 1069 | Н | LEU A | 76159.244 | -4.819 | 9.235 | 1.00 | 0.00 H | |
| ATOM | 1070 | HA | LEU A | 76159.597 | -3.794 | 6.595 | 1.00 | 0.00 H | |
| ATOM | 1071 | 1HB | LEU A | 76160.998 | -5.979 | 8.127 | 1.00 | 0.00 H | |
| ATOM | 1072 | 2HB | LEU A | 76161.469 | -5.483 | 6.513 | 1.00 | 0.00 H | |
| ATOM | 1073 | HG | LEU A | 76161.491 | -3.088 | 7.800 | 1.00 | 0.00 H | |
| ATOM | 1074 | 1HD1 | LEU A | 76161.129 | -4.740 | 9.897 | 1.00 | 0.00 H | |
| ATOM | 1075 | 2HD1 | LEU A | 76161.987 | -3.203 | 9.991 | 1.00 | 0.00 H | |
| ATOM | 1076 | 3HD1 | LEU A | 76162.890 | -4.708 | 9.819 | 1.00 | 0.00 H | |
| ATOM | 1077 | 1HD2 | LEU A | 76163.238 | -4.403 | 6.386 | 1.00 | 0.00 H | |
| ATOM | 1078 | 2HD2 | LEU A | 76163.903 | -4.844 | 7.959 | 1.00 | 0.00 H | |
| ATOM | 1079 | 3HD2 | LEU A | 76163.778 | -3.146 | 7.499 | 1.00 | 0.00 H | |
| ATOM | 1080 | N | LYS A | 77158.974 | -5.644 | 4.990 | 1.00 | 0.00 N | |
| ATOM | 1081 | CA | LYS A | 77158.350 | -6.593 | 4.075 | 1.00 | 0.00 C | |
| ATOM | 1082 | C | LYS A | 77156.836 | -6.610 | 4.257 | 1.00 | 0.00 C | |
| ATOM | 1083 | O | LYS A | 77156.193 | -7.648 | 4.097 | 1.00 | 0.00 O | |
| ATOM | 1084 | CB | LYS A | 77158.918 | -7.997 | 4.297 | 1.00 | 0.00 C | |
| ATOM | 1085 | CG | LYS A | 77160.436 | -8.038 | 4.345 | 1.00 | 0.00 C | |
| ATOM | 1086 | CD | LYS A | 77161.044 | -7.809 | 2.971 | 1.00 | 0.00 C | |
| ATOM | 1087 | CE | LYS A | 77162.497 | -7.372 | 3.069 | 1.00 | 0.00 C | |
| ATOM | 1088 | NZ | LYS A | 77163.335 | -7.988 | 2.004 | 1.00 | 0.00 N | |
| ATOM | 1089 | Н | LYS A | 77159.473 | -4.884 | 4.623 | 1.00 | 0.00 H | |

| ATOM | 1090 . | НА | LYS A | 77158.575 | -6.278 | 3.067 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|----------------|-------|------|--------|
| ATOM | 1091 1 | НВ | LYS A | 77158.538 | -8.382 | 5.231 | 1.00 | 0.00 H |
| ATOM | 1092 2 | 2HB | LYS A | 77158.587 | -8.637 | 3.492 | 1.00 | 0.00 H |
| ATOM | 1093 1 | HG | LYS A | 77160.787 | -7.268 | 5.015 | 1.00 | 0.00 H |
| ATOM | 1094 2 | HG | LYS A | 77160.749 | -9.005 | 4.710 | 1.00 | 0.00 H |
| ATOM | 1095 1 | HD | LYS A | 77160.993 | -8.729 | 2.407 | 1.00 | 0.00 H |
| ATOM | 1096 2 | 2HD | LYS A | 77160.480 | -7.041 | 2.462 | 1.00 | 0.00 H |
| ATOM | 1097 1 | HE | LYS A | 77162.544 | -6.298 | 2.975 | 1.00 | 0.00 H |
| ATOM | 1098 2 | HE | LYS A | 77162.883 | -7.667 | 4.034 | 1.00 | 0.00 H |
| ATOM | 1099 1 | HZ | LYS A | 77164.058 | -7.312 | 1.683 | 1.00 | 0.00 H |
| ATOM | 1100 2 | HZ | LYS A | 77162.743 | -8.255 | 1.192 | 1.00 | 0.00 H |
| ATOM | 1101 3 | HZ | LYS A | 77163.809 | -8.840 | 2.368 | 1.00 | 0.00 H |
| ATOM | 1102 | N | LYS A | 78156.273 | -5.453 | 4.593 | 1.00 | 0.00 N |
| ATOM | 1103 | CA | LYS A | 78154.833 | -5.336 | 4.796 | 1.00 | 0.00 C |
| ATOM | 1104 | C | LYS A | 78154.337 | -3.953 | 4.387 | 1.00 | 0.00 C |
| ATOM | 1105 | Ο | LYS A | 78153.462 | -3.379 | 5.035 | 1.00 | 0.00 O |
| ATOM | 1106 | CB | LYS A | 78154.482 | -5.606 | 6.260 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78154.975 | -6.951 | 6.768 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78154.548 | -7.196 | 8.206 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYS A | 78153.329 | -8.101 | 8.279 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78152.528 | -7.854 | 9.510 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78156.838 | - 4.661 | 4.705 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.350 | -6.076 | 4.177 | 1.00 | 0.00 H |
| ATOM | 1113 1 | НВ | LYS A | 78154.920 | -4.831 | 6.873 | 1.00 | 0.00 H |
| ATOM | 1114 2 | HB | LYS A | 78153.408 | -5.575 | 6.372 | 1.00 | 0.00 H |
| ATOM | 1115 1 | HG | LYS A | 78154.567 | -7.732 | 6.143 | 1.00 | 0.00 H |
| ATOM | 1116 2 | HG | LYS A | 78156.054 | -6.971 | 6.712 | 1.00 | 0.00 H |

| ATOM | 1117 1 | HD | LYS A | 78155.363 | -7.662 | 8.738 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1118 2 | HD | LYS A | 78154.310 | -6.247 | 8.667 | 1.00 | 0.00 H |
| ATOM | 1119 1 | HE | LYS A | 78152.709 | -7.919 | 7.414 | 1.00 | 0.00 H |
| ATOM | 1120 2 | HE | LYS A | 78153.660 | -9.129 | 8.274 | 1.00 | 0.00 H |
| ATOM | 1121 1 | HZ | LYS A | 78151.535 | -8.120 | 9.347 | 1.00 | 0.00 H |
| ATOM | 1122 2 | HZ | LYS A | 78152.568 | -6.849 | 9.768 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYS A | 78152.903 | -8.419 | 10.299 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79154.903 | -3.423 | 3.306 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.517 | -2.107 | 2.811 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.453 | -2.093 | 1.287 | 1.00 | 0.00 C |
| ATOM | 1127 | O | ALA A | 79155.479 | -1.991 | 0.614 | 1.00 | 0.00 O |
| ATOM | 1128 | CB | ALA A | 79155.491 | -1.050 | 3.310 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79155.595 | -3.929 | 2.832 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.538 | -1.876 | 3.204 | 1.00 | 0.00 H |
| ATOM | 1131 1 | HB | ALA A | 79154.952 | -0.139 | 3.526 | 1.00 | 0.00 H |
| ATOM | 1132 2 | 2HB | ALA A | 79156.234 | -0.858 | 2.551 | 1.00 | 0.00 H |
| ATOM | 1133 3 | BHB | ALA A | 79155.976 | -1.402 | 4.208 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.242 | -2.196 | 0.749 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.045 | -2.195 | -0.696 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.259 | -0.964 | -1.137 | 1.00 | 0.00 C |
| ATOM | 1137 | О | LEU A | 80151.060 | -0.857 | -0.880 | 1.00 | 0.00 O |
| ATOM | 1138 | CB | LEU A | 80152.312 | -3.465 | -1.132 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.003 | -3.553 | -2.627 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.212 | -4.072 | -3.391 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80150.795 | -4.445 | -2.870 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.462 | -2.275 | 1.338 | 1.00 | 0.00 H |
| ATOM | 1143 | HA | LEU A | 80154.018 | -2.173 | -1.164 | 1.00 | 0.00 H |

| ATOM | 1144 | 1HB | LEU A | 80152.919 | -4.317 | -0.859 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1145 | 2HB | LEU A | 80151.379 | -3.521 | -0.592 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.773 | -2.566 | -3.000 | 1.00 | 0.00 H |
| ATOM | 1147 | 1HD1 | LEU A | 80154.113 | -3.837 | -2.843 | 1.00 | 0.00 H |
| ATOM | 1148 | 2HD1 | LEU A | 80153.251 | -3.604 | -4.364 | 1.00 | 0.00 H |
| ATOM | 1149 | 3HD1 | LEU A | 80153.131 | -5.142 | -3.509 | 1.00 | 0.00 H |
| ATOM | 1150 | 1HD2 | LEU A | 80149.892 | -3.857 | -2.792 | 1.00 | 0.00 H |
| ATOM | 1151 | 2HD2 | LEU A | 80150.775 | -5.234 | -2.131 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80150.858 | -4.877 | -3.857 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.943 | -0.039 | -1.802 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.309 | 1.184 | -2.279 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.493 | 0.917 | -3.540 | 1.00 | 0.00 C |
| ATOM | 1156 | Ο | PHE A | 81151.877 | 0.102 | -4.379 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.364 | 2.255 | -2.559 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81154.090 | 2.718 | -1.328 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81155.218 | 2.048 | -0.880 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81153.645 | 3.822 | -0.619 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81155.888 | 2.471 | 0.252 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81154.311 | 4.250 | 0.515 | 1.00 | 0.00 C |
| ATOM | 1163 | CZ | PHE A | 81155.435 | 3.573 | 0.950 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.896 | -0.182 | -1.977 | 1.00 | 0.00 H |
| ATOM | 1165 | HA | PHE A | 81151.646 | 1.538 | -1.505 | 1.00 | 0.00 H |
| ATOM | 1166 | 1HB | PHE A | 81154.096 | 1.859 | -3.247 | 1.00 | 0.00 H |
| ATOM | 1167 | 2HB | PHE A | 81152.885 | 3.115 | -3.006 | 1.00 | 0.00 H |
| ATOM | 1168 | HD1 | PHE A | 81155.574 | 1.187 | -1.426 | 1.00 | 0.00 H |
| ATOM | 1169 | HD2 | PHE A | 81152.767 | 4.351 | -0.958 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81156.766 | 1.940 | 0.591 | 1.00 | 0.00 H |

| ATOM | 1171 | HE2 | PHE A | 81153.954 | 5.111 | 1.059 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 1172 | HZ | PHE A | 81155.957 | 3.906 | 1.835 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VALA | 82150.364 | 1.608 | -3.667 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VAL A | 82149.494 | 1.444 | -4.825 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VAL A | 82148.612 | 2.671 | -5.027 | 1.00 | 0.00 C |
| ATOM | 1176 | О | VAL A | 82148.497 | 3.519 | -4.142 | 1.00 | 0.00 O |
| ATOM | 1177 | СВ | VAL A | 82148.598 | 0.200 | -4.684 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VAL A | 82149.428 | -1.071 | -4.779 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VALA | 82147.827 | 0.243 | -3.373 | 1.00 | 0.00 C |
| ATOM | 1180 | Н | VAL A | 82150.111 | 2.242 | - 2.965 | 1.00 | 0.00 H |
| ATOM | 1181 | НА | VAL A | 82150.120 | 1.314 | -5.697 | 1.00 | 0.00 H |
| ATOM | . 1182 | HB | VAL A | 82147.885 | 0.200 | -5.496 | 1.00 | 0.00 H |
| ATOM | 1183 | 1HG1 | VAL A | 82150.036 | -1.038 | -5.671 | 1.00 | 0.00 H |
| ATOM | 1184 | 2HG1 | VAL A | 82148.771 | - 1.927 | -4.824 | 1.00 | 0.00 H |
| ATOM | 1185 | 3HG1 | VAL A | 82150.066 | -1.150 | -3.912 | 1.00 | 0.00 H |
| ATOM | 1186 | 1HG2 | VAL A | 82148.388 | 0.808 | -2.643 | 1.00 | 0.00 H |
| ATOM | 1187 | 2HG2 | VAL A | 82147.675 | -0.762 | -3.011 | 1.00 | 0.00 H |
| ATOM | 1188 | 3HG2 | VAL A | 82146.869 | 0.716 | -3.534 | 1.00 | 0.00 H |
| ATOM | 1189 | N | LYS A | 83147.991 | 2.760 | -6.199 | 1.00 | 0.00 N |
| ATOM | 1190 | CA | LYS A | 83147.118 | 3.884 | -6.518 | 1.00 | 0.00 C |
| ATOM | 1191 | C | LYS A | 83145.833 | 3.826 | -5.700 | 1.00 | 0.00 C |
| ATOM | 1192 | О | LYS A | 83145.108 | 2.831 | -5.732 | 1.00 | 0.00 O |
| ATOM | 1193 | CB | LYS A | 83146.786 | 3.890 | -8.012 | 1.00 | 0.00 C |
| ATOM | 1194 | CG | LYS A | 83148.004 | 4.058 | -8.904 | 1.00 | 0.00 C |
| ATOM | 1195 | CD | LYS A | 83147.623 | 4.036 | -10.376 | 1.00 | 0.00 C |
| ATOM | 1196 | CE | LYS A | 83148.408 | 5.068 | -11.171 | 1.00 | 0.00 C |
| ATOM | 1197 | NZ | LYS A | 83148.692 | 4.605 | -12.557 | 1.00 | 0.00 N |

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| ATOM | 1198 H | LYS A | 83148.122 | 2.052 | -6.864 | 1.00 | 0.00 H |
|------|-----------|-------|-----------|----------|--------|------|--------|
| ATOM | 1199 HA | LYS A | 83147.645 | 4.793 | -6.272 | 1.00 | 0.00 H |
| ATOM | 1200 1HB | LYS A | 83146.305 | 2.957 | -8.265 | 1.00 | 0.00 H |
| ATOM | 1201 2HB | LYS A | 83146.104 | 4.703 | -8.214 | 1.00 | 0.00 H |
| ATOM | 1202 1HG | LYS A | 83148.476 | 5.002 | -8.680 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.695 | 3.251 | -8.709 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83147.829 | 3.055 - | 10.778 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83146.568 | 4.250 - | 10.469 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83147.833 | 5.980 -1 | 1.217 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83149.343 | 5.258 -1 | 0.664 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83147.835 | 4.193 -1 | 2.979 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83149.440 | 3.882 -1 | 2.546 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83149.006 | 5.404 -1 | 3.143 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.559 | 4.900 | -4.967 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.362 | 4.977 | -4.138 | 1.00 | 0.00 C |
| ATOM | 1213 C | LEU A | 84143.103 | 4.813 | -4.985 | 1.00 | 0.00 C |
| ATOM | 1214 O | LEU A | 84142.124 | 4.210 | -4.547 | 1.00 | 0.00 O |
| ATOM | 1215 CB | LEU A | 84144.324 | 6.314 | -3.395 | 1.00 | 0.00 C |
| ATOM | 1216 CG | LEU A | 84143.055 | 6.569 | -2.580 | 1.00 | 0.00 C |
| ATOM | 1217 CD1 | LEU A | 84143.085 | 5.777 | -1.283 | 1.00 | 0.00 C |
| ATOM | 1218 CD2 | LEU A | 84142.896 | 8.055 | -2.295 | 1.00 | 0.00 C |
| ATOM | 1219 H | LEU A | 84146.177 | 5.660 | -4.986 | 1.00 | 0.00 H |
| ATOM | 1220 HA | LEU A | 84144.405 | 4.175 | -3.419 | 1.00 | 0.00 H |
| ATOM | 1221 1HB | LEU A | 84145.170 | 6.352 | -2.725 | 1.00 | 0.00 H |
| ATOM | 1222 2HB | LEU A | 84144.426 | 7.107 | -4.120 | 1.00 | 0.00 H |
| ATOM | 1223 HG | LEU A | 84142.197 | 6.243 | -3.150 | 1.00 | 0.00 H |
| ATOM | 1224 1HD1 | LEU A | 84142.799 | 4.753 | -1.479 | 1.00 | 0.00 H |

| ATOM | 1225 2HD1 | LEU A | 84142.394 | 6.214 | -0.577 | 1.00 | 0.00 H |
|------|-----------|-------|-----------|---------|---------|------|--------|
| ATOM | 1226 3HD1 | LEU A | 84144.083 | 5.798 | -0.870 | 1.00 | 0.00 H |
| ATOM | 1227 1HD2 | LEU A | 84143.784 | 8.425 | -1.805 | 1.00 | 0.00 H |
| ATOM | 1228 2HD2 | LEU A | 84142.040 | 8.209 | -1.654 | 1.00 | 0.00 H |
| ATOM | 1229 3HD2 | LEU A | 84142.750 | 8.586 | -3.224 | 1.00 | 0.00 H |
| ATOM | 1230 N | LYS A | 85143.138 | 5.352 | -6.199 | 1.00 | 0.00 N |
| ATOM | 1231 CA | LYS A | 85141.999 | 5.264 | -7.106 | 1.00 | 0.00 C |
| ATOM | 1232 C | LYS A | 85141.717 | 3.814 | -7.488 | 1.00 | 0.00 C |
| ATOM | 1233 O | LYSA | 85140.589 | 3.461 | -7.832 | 1.00 | 0.00 O |
| ATOM | 1234 CB | LYS A | 85142.259 | 6.093 | -8.365 | 1.00 | 0.00 C |
| ATOM | 1235 CG | LYS A | 85143.453 | 5.615 | -9.173 | 1.00 | 0.00 C |
| ATOM | 1236 CD | LYS A | 85143.781 | 6.575 | -10.306 | 1.00 | 0.00 C |
| ATOM | 1237 CE | LYS A | 85144.955 | 7.474 | -9.953 | 1.00 | 0.00 C |
| ATOM | 1238 NZ | LYS A | 85144.679 | 8.301 | -8.746 | 1.00 | 0.00 N |
| ATOM | 1239 H | LYS A | 85143.948 | 5.819 | -6.491 | 1.00 | 0.00 H |
| ATOM | 1240 HA | LYSA | 85141.137 | 5.662 | -6.595 | 1.00 | 0.00 H |
| ATOM | 1241 1HB | LYS A | 85141.384 | 6.050 | -8.997 | 1.00 | 0.00 H |
| ATOM | 1242 2HB | LYS A | 85142.433 | 7.118 | -8.077 | 1.00 | 0.00 H |
| ATOM | 1243 1HG | LYSA | 85144.310 | 5.538 | -8.521 | 1.00 | 0.00 H |
| ATOM | 1244 2HG | LYS A | 85143.229 | 4.643 | -9.590 | 1.00 | 0.00 H |
| ATOM | 1245 1HD | LYS A | 85144.031 | 6.004 | -11.188 | 1.00 | 0.00 H |
| ATOM | 1246 2HD | LYS A | 85142.914 | 7.189 | -10.506 | 1.00 | 0.00 H |
| ATOM | 1247 1HE | LYS A | 85145.821 | 6.858 | -9.766 | 1.00 | 0.00 H |
| ATOM | 1248 2HE | LYS A | 85145.154 | 8.129 - | 10.789 | 1.00 | 0.00 H |
| ATOM | 1249 1HZ | LYS A | 85145.546 | 8.784 | -8.437 | 1.00 | 0.00 H |
| ATOM | 1250 2HZ | LYS A | 85144.337 | 7.698 | -7.970 | 1.00 | 0.00 H |
| ATOM | 1251 3HZ | LYS A | 85143.953 | 9.015 | -8.959 | 1.00 | 0.00 H |

| ATOM | 1252 | N | SER A | 86142.750 | 2.976 | -7.427 | 1.00 | 0.00 N |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1253 | CA | SER A | 86142.608 | 1.565 | -7.767 | 1.00 | 0.00 C |
| ATOM | 1254 | C | SER A | 86142.494 | 0.710 | -6.509 | 1.00 | 0.00 C |
| ATOM | 1255 | O | SER A | 86142.923 | -0.444 | -6.490 | 1.00 | 0.00 O |
| ATOM | 1256 | СВ | SER A | 86143.800 | 1.100 | -8.607 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.657 | 1.500 | -9.959 | 1.00 | 0.00 O |
| ATOM | 1258 | Н | SER A | 86143.625 | 3.314 | -7.147 | 1.00 | 0.00 H |
| ATOM | 1259 | НА | SER A | 86141.704 | 1.453 | -8.347 | 1.00 | 0.00 H |
| ATOM | 1260 | HB | SER A | 86144.707 | 1.531 | -8.211 | 1.00 | 0.00 H |
| ATOM | 1261 2 | 2HB | SER A | 86143.866 | 0.023 | -8.568 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86143.468 | 2.440 | -9.997 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.913 | 1.284 | -5.460 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.742 | 0.575 | -4.198 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87140.267 | 0.304 | -3.923 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYS A | 87139.397 | 1.064 | -4.346 | 1.00 | 0.00 O |
| ATOM | 1267 | СВ | CYS A | 87142.347 | 1.382 | -3.048 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYSA | 87144.153 | 1.474 | -3.081 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYSA | 87141.592 | 2.207 | -5.537 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87142.262 | -0.369 | -4.274 | 1.00 | 0.00 H |
| ATOM | 1271 | 1HB | CYS A | 87141.968 | 2.393 | -3.089 | 1.00 | 0.00 H |
| ATOM | 1272 | 2HB | CYS A | 87142.057 | 0.933 | -2.110 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.471 | 1.371 | -2.181 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88139.992 | -0.786 | -3.212 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.620 | -1.156 | -2.882 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.440 | -1.289 | -1.372 | 1.00 | 0.00 C |
| ATOM | 1277 | О | ARG A | 88139.327 | -1.781 | -0.674 | 1.00 | 0.00 O |
| ATOM | 1278 | СВ | ARG A | 88138.247 | -2.472 | -3.569 | 1.00 | 0.00 C |
| | | | | | | | | |

| ATOM | 1279 | CG | ARG A | 88137.641 | -2.286 | -4.950 | 1.00 | 0.00 C |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1280 | CD | ARG A | 88136.123 | -2.374 | -4.909 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.530 | -2.222 | -6.236 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88135.476 | -1.068 | -6.897 | 1.00 | 0.00 C |
| ATOM | 1283 | NH1 | ARG A | 88135.977 | 0.037 | -6.359 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88134.919 | -1.019 | -8.099 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.729 | -1.354 | -2.903 | 1.00 | 0.00 H |
| ATOM | 1286 | НА | ARG A | 88137.971 | -0.374 | -3.246 | 1.00 | 0.00 H |
| ATOM | 1287 | 1HB | ARG A | 88139.136 | -3.077 | -3.669 | 1.00 | 0.00 H |
| ATOM | 1288 | 2HB | ARG A | 88137.533 | -2.997 | -2.953 | 1.00 | 0.00 H |
| ATOM | 1289 | 1HG | ARG A | 88137.924 | -1.316 | -5.330 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88138.019 | -3.056 | -5.606 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88135.842 | -3.335 | -4.507 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.749 | -1.591 | -4.265 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88135.152 | -3.023 | -6.656 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88136.399 | 0.007 | -5.453 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88135.934 | 0.901 | -6.861 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88134.539 | -1.848 | -8.509 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88134.878 | -0.152 | -8.596 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.282 | -0.854 | -0.841 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89136.995 | -0.931 | 0.595 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.153 | -2.347 | 1.140 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.565 | -3.293 | 0.616 | 1.00 | 0.00 O |
| ATOM | 1302 | CB | PRO A | 89135.534 | -0.482 | 0.696 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.303 | 0.344 | -0.521 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89136.166 | -0.254 | -1.596 | 1.00 | 0.00 C |
| ATOM | 1305 | НА | PRO A | 89137.622 | -0.257 | 1.160 | 1.00 | 0.00 H |
| | | | | | | | | |

| ATOM | 1306 1 | HB | PRO A | 89134.889 | -1.349 | 0.715 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|---------|------|--------|
| ATOM | 1307 2 | 2HB | PRO A | 89135.394 | 0.097 | 1.597 | 1.00 | 0.00 H |
| ATOM | 1308 1 | HG | PRO A | 89134.262 | 0.297 | - 0.805 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89135.596 | 1.367 | -0.332 | 1.00 | 0.00 H |
| ATOM | 1310 1 | HD | PRO A | 89135.619 | -1.009 | -2.142 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89136.522 | 0.515 | -2.265 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASP A | 90137.949 | - 2.484 | 2.196 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASPA | 90138.183 | -3.784 | 2.811 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.359 | -3.937 | 4.086 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASPA | 90137.749 | -3.455 | 5.149 | 1.00 | 0.00 O |
| ATOM | 1316 | СВ | ASP A | 90139.668 | -3.964 | 3.127 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90140.101 | -5.416 | 3.066 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASPA | 90139.932 | -6.041 | 1.997 | 1.00 | O 00.0 |
| ATOM | 1319 | OD2 | ASPA | 90140.609 | -5.928 | 4.085 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.389 | -1.691 | 2.569 | 1.00 | 0.00 H |
| ATOM | 1321 | НА | ASPA | 90137.878 | -4.544 | 2.107 | 1.00 | 0.00 H |
| ATOM | 1322 1 | HB | ASPA | 90140.253 | -3.403 | 2.413 | 1.00 | 0.00 H |
| ATOM | 1323 2 | 2HB | ASPA | 90139.866 | -3.589 | 4.120 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.220 | -4.611 | 3.972 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91135.343 | -4.826 | 5.118 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91135.563 | -6.209 | 5.723 | 1.00 | 0.00 C |
| ATOM | 1327 | O | SER A | 91134.646 | -6.803 | 6.289 | 1.00 | 0.00 O |
| ATOM | 1328 | CB | SER A | 91133.879 | -4.667 | 4.702 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91133.091 | -4.194 | 5.781 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91135.962 | -4.972 | 3.098 | 1.00 | 0.00 H |
| ATOM | 1331 | HA | SER A | 91135.579 | -4.079 | 5.859 | 1.00 | 0.00 H |
| ATOM | 1332 | 1HB | SER A | 91133.812 | -3.962 | 3.887 | 1.00 | 0.00 H |

| ATOM | 1333 2HI | B SER A | 91133.492 | -5.624 | 4.383 | 1.00 | 0.00 H |
|------|----------|----------|-------------|---------|-------|------|--------|
| ATOM | 1334 H | G SER A | 91132.300 | -4.732 | 5.861 | 1.00 | 0.00 H |
| ATOM | 1335 N | ARG A | 92136.787 | -6.715 | 5.600 | 1.00 | 0.00 N |
| ATOM | 1336 C | A ARGA | 92137.126 | -8.028 | 6.137 | 1.00 | 0.00 C |
| ATOM | 1337 C | ARG A | 92137.058 | -8.025 | 7.660 | 1.00 | 0.00 C |
| ATOM | 1338 O | ARG A | 92136.757 | -9.045 | 8.281 | 1.00 | 0.00 O |
| ATOM | 1339 C | B ARGA | 92138.525 | -8.444 | 5.677 | 1.00 | 0.00 C |
| ATOM | 1340 C | G ARGA | 92138.648 | -8.601 | 4.171 | 1.00 | 0.00 C |
| ATOM | 1341 C | D ARGA | 92137.984 | -9.879 | 3.686 | 1.00 | 0.00 C |
| ATOM | 1342 N | E ARGA | 92136.678 | -9.622 | 3.082 | 1.00 | 0.00 N |
| ATOM | 1343 C | Z ARGA | 92136.048 | -10.481 | 2.285 | 1.00 | 0.00 C |
| ATOM | 1344 N | H1 ARG A | 92136.599 | -11.654 | 1.994 | 1.00 | 0.00 N |
| ATOM | 1345 N | H2 ARG A | 92134.864 | -10.169 | 1.777 | 1.00 | 0.00 N |
| ATOM | 1346 H | I ARG A | 92137.477 | -6.195 | 5.139 | 1.00 | 0.00 H |
| ATOM | 1347 H | IA ARGA | 92136.406 | -8.738 | 5.757 | 1.00 | 0.00 H |
| ATOM | 1348 1H | B ARGA | 92139.234 | -7.696 | 5.999 | 1.00 | 0.00 H |
| ATOM | 1349 2H | B ARGA | 92138.776 | -9.388 | 6.138 | 1.00 | 0.00 H |
| ATOM | 1350 1H | G ARGA | 92138.176 | -7.758 | 3.690 | 1.00 | 0.00 H |
| ATOM | 1351 2H | G ARGA | 92139.696 | -8.627 | 3.906 | 1.00 | 0.00 H |
| ATOM | 1352 1H | D ARGA | 92138.623 | -10.346 | 2.952 | 1.00 | 0.00 H |
| ATOM | 1353 2H | D ARGA | 92137.856 | -10.545 | 4.527 | 1.00 | 0.00 H |
| ATOM | 1354 H | IE ARGA | 92136.248 | -8.764 | 3.281 | 1.00 | 0.00 H |
| ATOM | 1355 1H | H1 ARG A | 92137.492 - | -11.896 | 2.373 | 1.00 | 0.00 H |
| ATOM | 1356 2H | H1 ARG A | 92136.120 - | -12.295 | 1.395 | 1.00 | 0.00 H |
| ATOM | 1357 1H | H2 ARG A | 92134.444 | -9.288 | 1.993 | 1.00 | 0.00 H |
| ATOM | 1358 2H | H2 ARG A | 92134.390 - | -10.815 | 1.177 | 1.00 | 0.00 H |
| ATOM | 1359 N | PHE A | 93137.340 | -6.872 | 8.258 | 1.00 | 0.00 N |

| ATOM | 1360 | CA | PHE A | 93137.310 | -6.734 | 9.709 | 1.00 | 0.00 C | |
|--------|--------|-----|-------|-------------|---------|--------|------|--------|--|
| ATOM | 1361 | C | PHE A | 93136.350 | -5.627 | 10.133 | 1.00 | 0.00 C | |
| ATOM | 1362 | O | PHE A | 93136.554 | -4.973 | 11.155 | 1.00 | 0.00 O | |
| ATOM | 1363 | CB | PHE A | 93138.713 | -6.439 | 10.243 | 1.00 | 0.00 C | |
| ATOM · | 1364 | CG | PHE A | 93139.735 | -7.465 | 9.842 | 1.00 | 0.00 C | |
| ATOM | 1365 | CD1 | PHE A | 93140.148 | -7.570 | 8.523 | 1.00 | 0.00 C | |
| ATOM | 1366 | CD2 | PHE A | 93140.281 | -8.323 | 10.782 | 1.00 | 0.00 C | |
| ATOM | 1367 | CE1 | PHE A | 93141.090 | -8.512 | 8.151 | 1.00 | 0.00 C | |
| ATOM | 1368 | CE2 | PHE A | 93141.222 | -9.267 | 10.416 | 1.00 | 0.00 C | |
| ATOM | 1369 | CZ | PHE A | 93141.626 | -9.361 | 9.099 | 1.00 | 0.00 C | |
| ATOM | 1370 | Н | PHE A | 93137.572 | -6.093 | 7.709 | 1.00 | 0.00 H | |
| ATOM | 1371 | HA | PHE A | 93136.966 | -7.671 | 10.124 | 1.00 | 0.00 H | |
| ATOM | 1372 | lНВ | PHE A | 93139.039 | -5.481 | 9.867 | 1.00 | 0.00 H | |
| ATOM | 1373 2 | 2HB | PHE A | 93138.680 | -6.406 | 11.321 | 1.00 | 0.00 H | |
| ATOM | 1374 | HD1 | PHE A | 93139.731 | -6.905 | 7.782 | 1.00 | 0.00 H | |
| ATOM | 1375 | HD2 | PHE A | 93139.965 | -8.250 | 11.813 | 1.00 | 0.00 H | |
| ATOM | 1376 | HE1 | PHE A | 93141.403 | -8.585 | 7.120 | 1.00 | 0.00 H | |
| ATOM | 1377 | HE2 | PHE A | 93141.639 | -9.930 | 11.159 | 1.00 | 0.00 H | |
| ATOM | 1378 | HZ | PHE A | 93142.361 - | -10.099 | 8.811 | 1.00 | 0.00 H | |
| ATOM | 1379 | N | ALA A | 94135.303 | -5.421 | 9.339 | 1.00 | 0.00 N | |
| ATOM | 1380 | CA | ALAA | 94134.313 | -4.393 | 9.632 | 1.00 | 0.00 C | |
| ATOM | 1381 | C | ALAA | 94133.083 | -4.992 | 10.307 | 1.00 | 0.00 C | |
| ATOM | 1382 | Ο | ALA A | 94132.438 | -5.889 | 9.763 | 1.00 | 0.00 O | |
| ATOM | 1383 | CB | ALA A | 94133.918 | -3.663 | 8.357 | 1.00 | 0.00 C | |
| ATOM | 1384 | Н | ALA A | 94135.195 | -5.975 | 8.537 | 1.00 | 0.00 H | |
| ATOM | 1385 | НА | ALA A | 94134.765 | -3.677 | 10.302 | 1.00 | 0.00 H | |
| ATOM | 1386 | 1HB | ALA A | 94134.109 | -2.606 | 8.472 | 1.00 | 0.00 H | |

| ATOM | 1387 2H | IB ALAA | 94132.867 | -3.819 | 8.161 | 1.00 | 0.00 H |
|------|---------|-----------|-----------|--------|--------|------|--------|
| ATOM | 1388 3H | IB ALAA | 94134.498 | -4.044 | 7.530 | 1.00 | 0.00 H |
| ATOM | 1389 | N SER A | 95132.763 | -4.490 | 11.495 | 1.00 | 0.00 N |
| ATOM | 1390 | CA SERA | 95131.610 | -4.975 | 12.245 | 1.00 | 0.00 C |
| ATOM | 1391 | C SER A | 95130.308 | -4.529 | 11.587 | 1.00 | 0.00 C |
| ATOM | 1392 | O SER A | 95129.946 | -3.354 | 11.637 | 1.00 | 0.00 O |
| ATOM | 1393 | CB SER A | 95131.664 | -4.470 | 13.688 | 1.00 | 0.00 C |
| ATOM | 1394 | OG SER A | 95131.564 | -3.058 | 13.739 | 1.00 | 0.00 O |
| ATOM | 1395 J | H SER A | 95133.315 | -3.776 | 11.877 | 1.00 | 0.00 H |
| ATOM | 1396 I | HA SER A | 95131.648 | -6.054 | 12.249 | 1.00 | 0.00 H |
| ATOM | 1397 1F | IB SER A | 95130.845 | -4.897 | 14.247 | 1.00 | 0.00 H |
| ATOM | 1398 2F | IB SER A | 95132.600 | -4.770 | 14.136 | 1.00 | 0.00 H |
| ATOM | 1399 I | HG SER A | 95132.373 | -2.667 | 13.400 | 1.00 | 0.00 H |
| ATOM | 1400 | N LEUA | 96129.608 | -5.477 | 10.970 | 1.00 | 0.00 N |
| ATOM | 1401 | CA LEUA | 96128.346 | -5.182 | 10.302 | 1.00 | 0.00 C |
| ATOM | 1402 | C LEUA | 96127.436 | -6.404 | 10.293 | 1.00 | 0.00 C |
| ATOM | 1403 | O LEUA | 96126.247 | -6.309 | 10.601 | 1.00 | 0.00 O |
| ATOM | 1404 | CB LEUA | 96128.601 | -4.708 | 8.870 | 1.00 | 0.00 C |
| ATOM | 1405 | CG LEUA | 96127.648 | -3.623 | 8.366 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 LEU A | 96128.191 | -2.242 | 8.694 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 LEU A | 96127.421 | -3.768 | 6.869 | 1.00 | 0.00 C |
| ATOM | 1408 | H LEUA | 96129.949 | -6.395 | 10.965 | 1.00 | 0.00 H |
| ATOM | 1409 | HA LEUA | 96127.859 | -4.393 | 10.851 | 1.00 | 0.00 H |
| ATOM | 1410 1F | B LEU A | 96129.611 | -4.326 | 8.814 | 1.00 | 0.00 H |
| ATOM | 1411 2F | IB LEUA | 96128.520 | -5.561 | 8.212 | 1.00 | 0.00 H |
| ATOM | 1412 | HG LEUA | 96126.695 | -3.733 | 8.862 | 1.00 | 0.00 H |
| ATOM | 1413 1H | HD1 LEUA | 96129.269 | -2.255 | 8.634 | 1.00 | 0.00 H |

| ATOM | 1414 2HI | D1 LEU A | 96127.889 | -1.963 | 9.694 | 1.00 | 0.00 H |
|------|----------|----------|-------------|---------|--------|------|--------|
| ATOM | 1415 3HI | DI LEU A | 96127.801 | -1.524 | 7.987 | 1.00 | 0.00 H |
| ATOM | 1416 1HI | D2 LEU A | 96126.537 | -4.363 | 6.695 | 1.00 | 0.00 H |
| ATOM | 1417 2HI | D2 LEU A | 96128.275 | -4.253 | 6.421 | 1.00 | 0.00 H |
| ATOM | 1418 3HI | D2 LEU A | 96127.289 | -2.790 | 6.429 | 1.00 | 0.00 H |
| ATOM | 1419 N | GLN A | 97128.003 | -7.548 | 9.937 | 1.00 | 0.00 N |
| ATOM | 1420 C | A GLNA | 97127.247 | -8.794 | 9.885 | 1.00 | 0.00 C |
| ATOM | 1421 C | GLN A | 97126.955 | -9.315 | 11.292 | 1.00 | 0.00 C |
| ATOM | 1422 O | GLN A | 97125.796 | -9.457 | 11.681 | 1.00 | 0.00 O |
| ATOM | 1423 C | B GLN A | 97128.014 | -9.848 | 9.081 | 1.00 | 0.00 C |
| ATOM | 1424 C | G GLN A | 97127.274 | -10.326 | 7.843 | 1.00 | 0.00 C |
| ATOM | 1425 C | D GLN A | 97127.055 | -9.219 | 6.831 | 1.00 | 0.00 C |
| ATOM | 1426 O | E1 GLN A | 97127.736 | -8.193 | 6.859 | 1.00 | 0.00 O |
| ATOM | 1427 N | E2 GLN A | 97126.102 | -9.421 | 5.929 | 1.00 | 0.00 N |
| ATOM | 1428 H | GLN A | 97128.953 | -7.555 | 9.703 | 1.00 | 0.00 H |
| ATOM | 1429 H | A GLN A | 97126.309 | -8.591 | 9.390 | 1.00 | 0.00 H |
| ATOM | 1430 1HI | 3 GLN A | 97128.959 | -9.428 | 8.770 | 1.00 | 0.00 H |
| ATOM | 1431 2HI | 3 GLN A | 97128.202 | -10.703 | 9.714 | 1.00 | 0.00 H |
| ATOM | 1432 1HC | G GLN A | 97127.849 | -11.112 | 7.376 | 1.00 | 0.00 H |
| ATOM | 1433 2HG | G GLNA | 97126.311 | -10.716 | 8.143 | 1.00 | 0.00 H |
| ATOM | 1434 1HI | E2 GLN A | 97125.600 - | 10.262 | 5.967 | 1.00 | 0.00 H |
| ATOM | 1435 2HI | E2 GLN A | 97125.939 | -8.721 | 5.262 | 1.00 | 0.00 H |
| ATOM | 1436 N | PRO A | 98128.007 | -9.608 | 12.075 | 1.00 | 0.00 N |
| ATOM | 1437 C | A PRO A | 98127.855 | -10.116 | 13.442 | 1.00 | 0.00 C |
| ATOM | 1438 C | PRO A | 98127.388 | -9.036 | 14.412 | 1.00 | 0.00 C |
| ATOM | 1439 O | PRO A | 98127.027 | -7.933 | 14.001 | 1.00 | 0.00 O |
| ATOM | 1440 C | B PRO A | 98129.266 | -10.584 | 13.802 | 1.00 | 0.00 C |

| ATOM | 1441 CG | PRO A | 98130.167 | -9.736 | 12.973 | 1.00 | 0.00 C |
|------|----------|-------|-------------|---------|--------|------|--------|
| ATOM | 1442 CD | PRO A | 98129.426 | -9.470 | 11.691 | 1.00 | 0.00 C |
| ATOM | 1443 HA | PRO A | 98127.174 | -10.952 | 13.480 | 1.00 | 0.00 H |
| ATOM | 1444 1HB | PRO A | 98129.439 - | 10.434 | 14.858 | 1.00 | 0.00 H |
| ATOM | 1445 2HB | PRO A | 98129.375 - | 11.630 | 13.558 | 1.00 | 0.00 H |
| ATOM | 1446 1HG | PRO A | 98130.372 | -8.809 | 13.488 | 1.00 | 0.00 H |
| ATOM | 1447 2HG | PRO A | 98131.086 - | 10.266 | 12.772 | 1.00 | 0.00 H |
| ATOM | 1448 1HD | PRO A | 98129.634 | -8.470 | 11.337 | 1.00 | 0.00 H |
| ATOM | 1449 2HD | PRO A | 98129.695 - | 10.199 | 10.941 | 1.00 | 0.00 H |
| ATOM | 1450 N | SER A | 99127.397 | -9.361 | 15.700 | 1.00 | 0.00 N |
| ATOM | 1451 CA | SER A | 99126.974 | -8.420 | 16.730 | 1.00 | 0.00 C |
| ATOM | 1452 C | SER A | 99128.013 | -8.325 | 17.842 | 1.00 | 0.00 C |
| ATOM | 1453 O | SER A | 99127.894 | -8.984 | 18.875 | 1.00 | 0.00 O |
| ATOM | 1454 CB | SER A | 99125.624 | -8.841 | 17.313 | 1.00 | 0.00 C |
| ATOM | 1455 OG | SER A | 99125.449 | -10.245 | 17.232 | 1.00 | 0.00 O |
| ATOM | 1456 H | SER A | 99127.696 - | 10.257 | 15.965 | 1.00 | 0.00 H |
| ATOM | 1457 HA | SER A | 99126.869 | -7.449 | 16.269 | 1.00 | 0.00 H |
| ATOM | 1458 1HB | SER A | 99125.573 | -8.545 | 18.351 | 1.00 | 0.00 H |
| ATOM | 1459 2HB | SER A | 99124.830 | -8.359 | 16.762 | 1.00 | 0.00 H |
| ATOM | 1460 HG | SER A | 99125.229 | -10.489 | 16.329 | 1.00 | 0.00 H |
| ATOM | 1461 N | GLY A | 100129.034 | -7.502 | 17.623 | 1.00 | 0.00 N |
| ATOM | 1462 CA | GLY A | 100130.080 | -7.338 | 18.614 | 1.00 | 0.00 C |
| ATOM | 1463 C | GLY A | 100129.626 | -6.514 | 19.806 | 1.00 | 0.00 C |
| ATOM | 1464 O | GLY A | 100128.689 | -5.723 | 19.694 | 1.00 | 0.00 O |
| ATOM | 1465 H | GLY A | 100129.076 | -7.003 | 16.780 | 1.00 | 0.00 H |
| ATOM | 1466 1HA | GLY A | 100130.389 | -8.312 | 18.962 | 1.00 | 0.00 H |
| ATOM | 1467 2HA | GLY A | 100130.925 | -6.847 | 18.153 | 1.00 | 0.00 H |

| ATOM | 1468 | N | PRO A 101130.277 | -6.678 | 20.969 | 1.00 | 0.00 N |
|------|--------|-----|------------------|--------|--------|------|--------|
| ATOM | 1469 | CA | PRO A 101129.924 | -5.935 | 22.183 | 1.00 | 0.00 C |
| ATOM | 1470 | C | PRO A 101130.281 | -4.456 | 22.081 | 1.00 | 0.00 C |
| ATOM | 1471 | О | PRO A 101130.835 | -4.008 | 21.078 | 1.00 | 0.00 O |
| ATOM | 1472 | СВ | PRO A 101130.760 | -6.613 | 23.272 | 1.00 | 0.00 C |
| ATOM | 1473 | CG | PRO A 101131.923 | -7.196 | 22.548 | 1.00 | 0.00 C |
| ATOM | 1474 | CD | PRO A 101131.408 | -7.600 | 21.194 | 1.00 | 0.00 C |
| ATOM | 1475 | НА | PRO A 101128.874 | -6.036 | 22.418 | 1.00 | 0.00 H |
| ATOM | 1476 1 | НВ | PRO A 101131.075 | -5.877 | 23.998 | 1.00 | 0.00 H |
| ATOM | 1477 2 | 2HB | PRO A 101130.173 | -7.379 | 23.757 | 1.00 | 0.00 H |
| ATOM | 1478 1 | HG | PRO A 101132.702 | -6.456 | 22.446 | 1.00 | 0.00 Ḥ |
| ATOM | 1479 2 | 2HG | PRO A 101132.292 | -8.060 | 23.080 | 1.00 | 0.00 H |
| ATOM | 1480 1 | HD | PRO A 101132.171 | -7.462 | 20.442 | 1.00 | 0.00 H |
| ATOM | 1481 2 | 2HD | PRO A 101131.071 | -8.625 | 21.207 | 1.00 | 0.00 H |
| ATOM | 1482 | N | SER A 102129.959 | -3.702 | 23.127 | 1.00 | 0.00 N |
| ATOM | 1483 | CA | SER A 102130.245 | -2.272 | 23.156 | 1.00 | 0.00 C |
| ATOM | 1484 | C | SER A 102131.024 | -1.897 | 24.413 | 1.00 | 0.00 C |
| ATOM | 1485 | O | SER A 102132.035 | -1.200 | 24.344 | 1.00 | 0.00 O |
| ATOM | 1486 | CB | SER A 102128.945 | -1.469 | 23.089 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102127.980 | -2.124 | 22.284 | 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102129.518 | -4.116 | 23.899 | 1.00 | 0.00 H |
| ATOM | 1489 | HA | SER A 102130.847 | -2.037 | 22.291 | 1.00 | 0.00 H |
| ATOM | 1490 1 | HB | SER A 102128.544 | -1.353 | 24.086 | 1.00 | 0.00 H |
| ATOM | 1491 2 | 2HB | SER A 102129.146 | -0.495 | 22.668 | 1.00 | 0.00 H |
| ATOM | 1492 | HG | SER A 102128.380 | -2.382 | 21.450 | 1.00 | 0.00 H |
| ATOM | 1493 | N | SER A 103130.545 | -2.367 | 25.561 | 1.00 | 0.00 N |
| ATOM | 1494 | CA | SER A 103131.197 | -2.082 | 26.834 | 1.00 | 0.00 C |

SER A 103130.874 -3.160 27.863 **ATOM** 1495 C 1.00 0.00 C **ATOM** 1496 Ο SER A 103131.771 -3.823 28.384 1.00 0.00 O **ATOM** 1497 CB SER A 103130.760 -0.712 27.358 1.00 0.00 C SER A 103131.620 0.311 1.00 0.00 O **ATOM** 1498 OG 26.891 SER A 103129.734 -2.918 25.551 1.00 0.00 H **ATOM** 1499 Η **ATOM** 1500 HA SER A 103132.262 -2.069 26.665 1.00 0.00 H SER A 103129.756 -0.503 27.021 **ATOM** 1501 1HB 1.00 0.00 H SER A 103130.783 -0.720 28.438 1.00 0.00 H 1502 2HB **ATOM** SER A 103132.396 0.360 27.455 1.00 0.00 H **ATOM** 1503 HG -3.329 28.153 1.00 0.00 N 1504 N GLY A 104129.588 **ATOM ATOM** 1505 $\mathsf{C}\mathsf{A}$ GLY A 104129.170 -4.328 29.119 1.00 0.00 C **ATOM** 1506 C GLY A 104127.832 -4.001 29.751 1.00 0.00 C 1507 -3.345 30.815 1.00 0.00 O **ATOM** O GLY A 104127.823 **ATOM** 1508 OXT GLY A 104126.794 -4.397 29.183 1.00 0.00 O GLY A 104128.917 -2.771 27.707 1.00 0.00 H **ATOM** 1509 H 1510 1HA GLY A 104129.097 -5.284 28.622 1.00 0.00 H **ATOM** 1511 2HA GLY A 104129.917 -4.395 29.897 1.00 0.00 H **ATOM** 1512 GLY A 104 TER

ENDMDL

Three-Dimensional Structure Coordinate Table 8

ATOM 1 N GLY A 1.00 0.00 N 1135.862 21.326 -5.428 1136.784 22.453 -5.740 1.00 0.00 C ATOM 2 CA GLY A 1136.436 23.144 -7.044 1.00 0.00 C ATOM 3 C GLY A 1135.778 24.184 -7.046 1.00 0.00 O ATOM 4 O GLY A 1134.965 21.447 -5.941 1.00 0.00 H ATOM 5 1H GLY A 1135.664 21.298 -4.408 1.00 0.00 H ATOM 6 2H GLY A

| ATOM 7 3 | H | GLY A | 1136.294 | 20.423 | -5.712 | 1.00 | 0.00 H | |
|----------|-----|-------|----------|--------|---------|------|--------|--|
| ATOM 8 1 | HA | GLY A | 1136.736 | 23.175 | -4.938 | 1.00 | 0.00 H | |
| ATOM 9 2 | HA | GLY A | 1137.793 | 22.071 | -5.805 | 1.00 | 0.00 H | |
| ATOM10 | N | SER A | 2136.880 | 22.565 | -8.154 | 1.00 | 0.00 N | |
| ATOM11 | CA | SER A | 2136.611 | 23.132 | -9.471 | 1.00 | 0.00 C | |
| ATOM12 | C | SER A | 2135.133 | 23.008 | -9.825 | 1.00 | 0.00 C | |
| ATOM13 | О | SER A | 2134.622 | 21.906 | -10.024 | 1.00 | 0.00 O | |
| ATOM14 | СВ | SER A | 2137.463 | 22.432 | -10.532 | 1.00 | 0.00 C | |
| ATOM15 | OG | SER A | 2137.904 | 23.351 | -11.518 | 1.00 | 0.00 O | |
| ATOM16 | Н | SER A | 2137.399 | 21.736 | -8.087 | 1.00 | 0.00 H | |
| ATOM17 | НА | SER A | 2136.876 | 24.178 | -9.441 | 1.00 | 0.00 H | |
| ATOM18 | НВ | SER A | 2138.326 | 21.986 | -10.063 | 1.00 | 0.00 H | |
| ATOM19 2 | 2HB | SER A | 2136.876 | 21.663 | -11.012 | 1.00 | 0.00 H | |
| ATOM20 | HG | SER A | 2138.856 | 23.456 | -11.454 | 1.00 | 0.00 H | |
| ATOM21 | N | SER A | 3134.452 | 24.146 | -9.904 | 1.00 | 0.00 N | |
| ATOM22 | CA | SER A | 3133.032 | 24.166 | -10.234 | 1.00 | 0.00 C | |
| ATOM23 | C | SER A | 3132.822 | 24.039 | -11.740 | 1.00 | 0.00 C | |
| ATOM24 | О | SER A | 3133.076 | 24.979 | -12.494 | 1.00 | 0.00 O | |
| ATOM25 | СВ | SER A | 3132.385 | 25.455 | -9.725 | 1.00 | 0.00 C | |
| ATOM26 | OG | SER A | 3132.929 | 26.590 | -10.375 | 1.00 | 0.00 O | |
| ATOM27 | Н | SER A | 3134.915 | 24.993 | -9.735 | 1.00 | 0.00 H | |
| ATOM28 | HA | SER A | 3132.567 | 23.323 | -9.747 | 1.00 | 0.00 H | |
| ATOM29 | НВ | SER A | 3131.323 | 25.422 | -9.915 | 1.00 | 0.00 H | |
| ATOM30 2 | 2НВ | SER A | 3132.558 | 25.547 | -8.663 | 1.00 | 0.00 H | |
| ATOM31 | HG | SER A | 3132.626 | 26.615 | -11.286 | 1.00 | 0.00 H | |
| ATOM32 | N | GLY A | 4132.358 | 22.871 | -12.172 | 1.00 | 0.00 N | |
| ATOM33 | CA | GLY A | 4132.122 | 22.643 | -13.585 | 1.00 | 0.00 C | |

| | | | | - 442 - | | |
|----------|-----|-------|----------|----------------|------|--------|
| ATOM34 | С | GLY A | 4132.095 | 21.169 -13.938 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4132.285 | 20.314 -13.073 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4132.174 | 22.159 -11.525 | 1.00 | 0.00 H |
| ATOM37 1 | НА | GLY A | 4131.175 | 23.084 -13.857 | 1.00 | 0.00 H |
| ATOM38 2 | 2HA | GLY A | 4132.906 | 23.123 -14.151 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5131.857 | 20.871 -15.211 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5131.806 | 19.490 -15.676 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5130.700 | 18.717 -14.963 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5130.136 | 19.190 -13.977 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5133.153 | 18.803 -15.448 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5133.460 | 17.916 -16.510 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5131.714 | 21.598 -15.853 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5131.593 | 19.505 -16.734 | 1.00 | 0.00 H |
| ATOM47 | lНВ | SER A | 5133.930 | 19.550 -15.385 | 1.00 | 0.00 H |
| ATOM48 2 | 2HB | SER A | 5133.118 | 18.242 -14.526 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5133.809 | 18.414 -17.252 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6130.397 | 17.527 -15.469 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6129.360 | 16.689 -14.880 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6129.754 | 15.216 -14.934 | 1.00 | 0.00 C |
| ATOM53 | Ο | SER A | 6129.519 | 14.536 -15.934 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6128.031 | 16.900 -15.608 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6128.003 | 18.156 -16.264 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6130.884 | 17.203 -16.256 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6129.244 | 16.980 -13.847 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6127.897 | 16.121 -16.343 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6127.222 | 16.863 -14.893 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6127.925 | 18.856 -15.612 | 1.00 | 0.00 H |

| ATOM61 | N | GLY A | 7130.352 | 14.729 - | 13.853 | 1.00 | 0.00 N |
|--------|------|-------|----------|----------|---------|------|--------|
| ATOM62 | CA | GLY A | 7130.769 | 13.340 - | 13.798 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7131.372 | 12.967 - | 12.458 | 1.00 | 0.00 C |
| ATOM64 | O | GLY A | 7132.589 | 12.825 - | 12.335 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7130.513 | 15.317 - | 13.085 | 1.00 | 0.00 H |
| ATOM66 | lΗA | GLY A | 7129.910 | 12.711 - | 13.981 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7131.502 | 13.165 - | 14.571 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8130.520 | 12.809 - | 11.450 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8130.974 | 12.451 | -10.112 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8130.399 | 11.105 | -9.684 | 1.00 | 0.00 C |
| ATOM71 | О | LEU A | 8129.312 | 10.718 - | 10.114 | 1.00 | 0.00 O |
| ATOM72 | СВ | LEU A | 8130.573 | 13.532 | -9.107 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8130.735 | 14.970 | -9.605 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8129.892 | 15.921 | -8.770 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8132.199 | 15.382 | -9.570 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8129.561 | 12.936 - | -11.611 | 1.00 | 0.00 H |
| ATOM77 | НА | LEU A | 8132.051 | 12.376 | -10.136 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8129.538 | 13.379 | -8.841 | 1.00 | 0.00 H |
| ATOM79 | 2HB | LEU A | 8131.177 | 13.412 | -8.221 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8130.392 | 15.031 | -10.627 | 1.00 | 0.00 H |
| ATOM81 | 1HD1 | LEU A | 8129.871 | 16.892 | -9.242 | 1.00 | 0.00 H |
| ATOM82 | 2HD1 | LEU A | 8130.321 | 16.010 | -7.782 | 1.00 | 0.00 H |
| ATOM83 | 3HD1 | LEU A | 8128.885 | 15.537 | -8.692 | 1.00 | 0.00 H |
| ATOM84 | 1HD2 | LEU A | 8132.656 | 15.168 - | 10.525 | 1.00 | 0.00 H |
| ATOM85 | 2HD2 | LEU A | 8132.710 | 14.832 | -8.795 | 1.00 | 0.00 H |
| ATOM86 | 3HD2 | LEU A | 8132.270 | 16.441 | -9.367 | 1.00 | 0.00 H |
| ATOM87 | N | ALA A | 9131.134 | 10.395 | -8.834 | 1.00 | 0.00 N |

| ATOM88 | CA | ALA | A | 913 | 0.696 | 9.09 | 2 -8.3 | 348 | 1.00 | 0.00 | C |
|-------------------|-----|-----|----|-------|-------|-------|----------|------------|-------|--------|--------|
| ATOM89 | C | ALA | Α | 9131 | 1.453 | 8.69 | 4 -7.0 | 86 | 1.00 | 0.00 | С |
| ATOM90 | O | ALA | Α | 913 | 1.772 | 7.52 | 2 -6.8 | 86 | 1.00 | 0.00 | О |
| ATOM91 | СВ | ALA | A | 913 | 0.878 | 8.03 | 8 -9.4 | 130 | 1.00 | 0.00 | C |
| ATOM92 | Н | ALA | Α | 913 | 1.991 | 10.75 | 6 -8.5 | 27 | 1.00 | 0.00 | Н |
| ATOM93 | НА | ALA | A | 912 | 9.643 | 9.16 | 0 -8. | 118 | 1.00 | 0.00 | Н |
| ATOM94 1 | НВ | ALA | Α | 9129 | 9.990 | 7.99 | 5 -10.04 | 4 5 | 1.00 | 0.00 H | Ŧ |
| ATOM95 2 | HB | ALA | Α | 9131 | .042 | 7.07 | 5 -8.9 | 70 | 1.00 | 0.00 | Н |
| ATOM96 3 | HB | ALA | Α | 9131 | .728 | 8.29 | 5 -10.04 | 14 | 1.00 | 0.00 H | 1 |
| ATOM97 | N | MET | A | 1013 | 1.737 | 9.67 | 5 -6.2 | 238 | 1.00 | 0.00 | N |
| ATOM98 | CA | MET | ſΑ | 1013 | 2.457 | 9.42 | 7 -4.9 | 994 | 1.00 | 0.00 | C |
| ATOM99 | C | MET | A | 10132 | 2.314 | 10.60 | 8 -4.0 |)35 | 1.00 | 0.00 | С |
| ATOM | 100 | O | ME | TA | 10133 | 3.291 | 11.291 | -3 | .728 | 1.00 | 0.00 O |
| ATOM | 101 | CB | ME | ET A | 10133 | 3.936 | 9.159 | -: | 5.280 | 1.00 | 0.00 C |
| ATOM | 102 | CG | MI | ET A | 1013 | 4.602 | 10.24 | 8 -(| 5.106 | 1.00 | 0.00 C |
| ATOM | 103 | SD | ME | ET A | 10136 | 5.400 | 10.200 |) -5 | 5.997 | 1.00 | 0.00 S |
| ATOM | 104 | CE | ME | ETA | 10136 | 5.829 | 11.766 | 5 -6 | 5.751 | 1.00 | 0.00 C |
| ATOM | 105 | Н | ME | TA | 10131 | .456 | 10.589 |) -6 | 5.452 | 1.00 | 0.00 H |
| ATOM | 106 | HA | MI | ET A | 1013 | 2.025 | 8.55 | 0 - | 4.532 | 1.00 | 0.00 H |
| ATOM | 107 | 1HB | ME | TA | 10134 | .463 | 9.076 | - 4 | .342 | 1.00 | 0.00 H |
| ATOM | 108 | 2HB | ME | TA | 10134 | .023 | 8.226 | 5 -5 | .817 | 1.00 | 0.00 H |
| ATOM | 109 | 1HG | ME | TA | 10134 | 1.315 | 10.123 | 3 -7 | 7.140 | 1.00 | 0.00 H |
| ATOM | 110 | 2HG | ME | TA | 10134 | 1.259 | 11.209 | -5 | 5.752 | 1.00 | 0.00 H |
| ATOM | 111 | 1HE | ME | ΤA | 10137 | .179 | 11.598 | -7 | .758 | 1.00 | 0.00 H |
| ATOM ⁻ | 112 | 2HE | ME | ΤA | 10137 | .606 | 12.244 | - 6 | .174 | 1.00 | 0.00 H |
| ATOM | 113 | 3HE | ME | TA | 10135 | .957 | 12.404 | -6 | .776 | 1.00 | 0.00 H |
| ATOM | 114 | N | PR | ΟA | 11131 | .087 | 10.866 | -3 | .550 | 1.00 | 0.00 N |

| ATOM | 115 | CA | PRO A | 11130.821 | 11.971 | -2.624 | 1.00 | 0.00 C |
|------|---------|----|-------|-----------|--------|--------|------|--------|
| ATOM | 116 | C | PRO A | 11131.642 | 11.867 | -1.340 | 1.00 | 0.00 C |
| ATOM | 117 | О | PRO A | 11132.251 | 12.845 | -0.908 | 1.00 | 0.00 O |
| ATOM | 118 | СВ | PRO A | 11129.326 | 11.848 | -2.315 | 1.00 | 0.00 C |
| ATOM | 119 | CG | PRO A | 11128.762 | 11.010 | -3.412 | 1.00 | 0.00 C |
| ATOM | 120 | CD | PRO A | 11129.869 | 10.103 | -3.867 | 1.00 | 0.00 C |
| ATOM | 121 | HA | PRO A | 11131.015 | 12.926 | -3.092 | 1.00 | 0.00 H |
| ATOM | 122 11 | НВ | PRO A | 11129.192 | 11.379 | -1.351 | 1.00 | 0.00 H |
| ATOM | 123 21 | НВ | PRO A | 11128.878 | 12.831 | -2.304 | 1.00 | 0.00 H |
| ATOM | 124 11 | HG | PRO A | 11127.936 | 10.427 | -3.036 | 1.00 | 0.00 H |
| ATOM | 125 21 | HG | PRO A | 11128.436 | 11.641 | -4.225 | 1.00 | 0.00 H |
| ATOM | 126 11 | HD | PRO A | 11129.843 | 9.171 | -3.321 | 1.00 | 0.00 H |
| ATOM | 127 21 | HD | PRO A | 11129.794 | 9.920 | -4.929 | 1.00 | 0.00 H |
| ATOM | 128 | N | PRO A | 12131.677 | 10.677 | -0.709 | 1.00 | 0.00 N |
| ATOM | 129 | CA | PRO A | 12132.438 | 10.469 | 0.528 | 1.00 | 0.00 C |
| ATOM | 130 | C | PRO A | 12133.904 | 10.857 | 0.370 | 1.00 | 0.00 C |
| ATOM | 131 | О | PRO A | 12134.589 | 11.145 | 1.352 | 1.00 | 0.00 O |
| ATOM | 132 | CB | PRO A | 12132.309 | 8.965 | 0.784 | 1.00 | 0.00 C |
| ATOM | 133 | CG | PRO A | 12131.074 | 8.556 | 0.061 | 1.00 | 0.00 C |
| ATOM | 134 | CD | PRO A | 12130.989 | 9.447 | -1.146 | 1.00 | 0.00 C |
| ATOM | 135 | HA | PRO A | 12132.008 | 11.017 | 1.353 | 1.00 | 0.00 H |
| ATOM | 136 11 | HB | PRO A | 12133.180 | 8.455 | 0.397 | 1.00 | 0.00 H |
| ATOM | 137 21 | HB | PRO A | 12132.223 | 8.783 | 1.845 | 1.00 | 0.00 H |
| ATOM | -138 11 | HG | PRO A | 12131.149 | 7.522 | -0.240 | 1.00 | 0.00 H |
| ATOM | 139 21 | HG | PRO A | 12130.212 | 8.703 | 0.695 | 1.00 | 0.00 H |
| ATOM | 140 11 | HD | PRO A | 12131.501 | 8.996 | -1.984 | 1.00 | 0.00 H |
| ATOM | 141 21 | HD | PRO A | 12129.959 | 9.647 | -1.395 | 1.00 | 0.00 H |

| ATOM | 142 | N | GLY A | 13134.378 | 10.862 | -0.872 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 143 | CA | GLY A | 13135.761 | 11.216 | -1.136 | 1.00 | 0.00 C |
| ATOM | 144 | C | GLY A | 13136.420 | 10.278 | -2.127 | 1.00 | 0.00 C |
| ATOM | 145 | O | GLY A | 13136.953 | 10.716 | -3.146 | 1.00 | 0.00 O |
| ATOM | 146 | Н | GLY A | 13133.785 | 10.624 | -1.616 | 1.00 | 0.00 H |
| ATOM | 147 | 1HA | GLY A | 13135.794 | 12.220 | -1.531 | 1.00 | 0.00 H |
| ATOM | 148 2 | 2HA | GLY A | 13136.311 | 11.187 | -0.208 | 1.00 | 0.00 H |
| ATOM | 149 | N | ASN A | 14136.385 | 8.983 | -1.827 | 1.00 | 0.00 N |
| ATOM | 150 | CA | ASN A | 14136.984 | 7.980 | -2.698 | 1.00 | 0.00 C |
| ATOM | 151 | C | ASN A | 14136.171 | 6.690 | -2.683 | 1.00 | 0.00 C |
| ATOM | 152 | О | ASN A | 14136.322 | 5.861 | -1.785 | 1.00 | 0.00 O |
| ATOM | 153 | CB | ASN A | 14138.424 | 7.694 | -2.268 | 1.00 | 0.00 C |
| ATOM | 154 | CG | ASN A | 14139.315 | 8.916 | -2.382 | 1.00 | 0.00 C |
| ATOM | 155 | OD1 | ASN A | 14140.077 | 9.056 | -3.338 | 1.00 | 0.00 O |
| ATOM | 156 | ND2 | ASN A | 14139.222 | 9.809 | -1.403 | 1.00 | 0.00 N |
| ATOM | 157 | Н | ASN A | 14135.946 | 8.697 | -0.999 | 1.00 | 0.00 H |
| ATOM | 158 | НА | ASN A | 14136.990 | 8.375 | -3.704 | 1.00 | 0.00 H |
| ATOM | 159 | 1HB | ASN A | 14138.428 | 7.364 | -1.240 | 1.00 | 0.00 H |
| ATOM | 160 | 2HB | ASN A | 14138.832 | 6.914 | -2.894 | 1.00 | 0.00 H |
| ATOM | 161 | 1HD2 | ASN A | 14138.593 | 9.631 | -0.673 | 1.00 | 0.00 H |
| ATOM | 162 | 2HD2 | ASN A | 14139.787 | 10.609 | -1.451 | 1.00 | 0.00 H |
| ATOM | 163 | N | SER A | 15135.310 | 6.527 | -3.682 | 1.00 | 0.00 N |
| ATOM | 164 | CA | SER A | 15134.470 | 5.338 | -3.787 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15133.494 | 5.253 | -2.616 | 1.00 | 0.00 C |
| ATOM | 166 | О | SER A | 15132.317 | 5.585 | -2.753 | 1.00 | 0.00 O |
| ATOM | 167 | СВ | SER A | 15135.336 | 4.076 | -3.840 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15135.576 | 3.678 | -5.179 | 1.00 | 0.00 O |

| ATOM | 169 | Н | SER A | 15135.237 | 7.224 | -4.368 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 170 | НА | SER A | 15133.905 | 5.413 | -4.704 | 1.00 | 0.00 H |
| ATOM | 171 1 | HB | SER A | 15136.284 | 4.272 | -3.361 | 1.00 | 0.00 H |
| ATOM | 172 2 | HB | SER A | 15134.832 | 3.273 | -3.323 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15136.355 | 4.129 | -5.512 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16133.990 | 4.808 | -1.466 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.161 | 4.680 | -0.273 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16133.758 | 5.463 | 0.892 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.046 | 6.158 | 1.616 | 1.00 | 0.00 O |
| ATOM | 178 | СВ | HIS A | 16133.007 | 3.208 | 0.111 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16131.982 | 2.480 | -0.703 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16130.635 | 2.772 | -0.652 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16132.113 | 1.469 | -1.593 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16129.982 | 1.969 | -1.475 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16130.856 | 1.170 | -2.059 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16134.936 | 4.559 | -1.419 | 1.00 | 0.00 H |
| ATOM | 185 | НА | HIS A | 16132.187 | 5.087 | -0.502 | 1.00 | 0.00 H |
| ATOM | 186 1 | НВ | HIS A | 16133.953 | 2.708 | -0.024 | 1.00 | 0.00 H |
| ATOM | 187 2 | HB | HIS A | 16132.715 | 3.143 | 1.149 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16130.219 | 3.462 | -0.095 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HIS A | 16133.035 | 0.986 | -1.884 | 1.00 | 0.00 H |
| ATOM | 190 | HE1 | HIS A | 16128.915 | 1.969 | -1.642 | 1.00 | 0.00 H |
| ATOM | 191 | HE2 | HIS A | 16130.650 | 0.540 | -2.779 | 1.00 | 0.00 H |
| ATOM | 192 | N | GLY A | 17135.070 | 5.345 | 1.066 | 1.00 | 0.00 N |
| ATOM | 193 | CA | GLY A | 17135.741 | 6.047 | 2.144 | 1.00 | 0.00 C |
| ATOM | 194 | C | GLY A | 17137.087 | 5.436 | 2.485 | 1.00 | 0.00 C |
| ATOM | 195 | О | GLY A | 17137.242 | 4.806 | 3.530 | 1.00 | 0.00 O |

| ATOM | 196 | Н | GLY A | 17135.587 | 4.777 | 0.457 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|-------|--------|------|--------|
| ATOM | 197 | 1HA | GLY A | 17135.889 | 7.076 | 1.853 | 1.00 | 0.00 H |
| ATOM | 198 2 | 2HA | GLY A | 17135.113 | 6.019 | 3.022 | 1.00 | 0.00 H |
| ATOM | 199 | N | LEU A | 18138.060 | 5.623 | 1.600 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.399 | 5.086 | 1.811 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.344 | 6.167 | 2.328 | 1.00 | 0.00 C |
| ATOM | 202 | О | LEU A | 18140.685 | 7.103 | 1.606 | 1.00 | 0.00 O |
| ATOM | 203 | СВ | LEU A | 18139.946 | 4.493 | 0.511 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18139.060 | 3.428 | -0.138 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18139.482 | 3.188 | -1.579 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18139.115 | 2.134 | 0.659 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18137.874 | 6.134 | 0.784 | 1.00 | 0.00 H |
| ATOM | 208 | HA | LEU A | 18139.328 | 4.303 | 2.551 | 1.00 | 0.00 H |
| ATOM | 209 | 1HB | LEU A | 18140.082 | 5.298 | -0.196 | 1.00 | 0.00 H |
| ATOM | 210 | 2HB | LEU A | 18140.908 | 4.051 | 0.718 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18138.037 | 3.776 | -0.144 | 1.00 | 0.00 H |
| ATOM | 212 | 1HD1 | LEU A | 18139.230 | 2.178 | -1.864 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18140.549 | 3.332 | -1.670 | 1.00 | 0.00 H |
| ATOM | 214 | 3HD1 | LEU A | 18138.969 | 3.883 | -2.226 | 1.00 | 0.00 H |
| ATOM | 215 | 1HD2 | LEU A | 18140.134 | 1.935 | 0.954 | 1.00 | 0.00 H |
| ATOM | 216 | 2HD2 | LEU A | 18138.751 | 1.320 | 0.050 | 1.00 | 0.00 H |
| ATOM | 217 | 3HD2 | LEU A | 18138.497 | 2.226 | 1.540 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19140.763 | 6.029 | 3.581 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19141.670 | 6.993 | 4.194 | 1.00 | 0.00 C |
| ATOM | 220 | C | GLU A | 19142.671 | 6.294 | 5.108 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19142.581 | 5.089 | 5.338 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19140.878 | 8.036 | 4.986 | 1.00 | 0.00 C |

| ATOM | 223 | CG | GLU A | 19139.943 | 7.432 | 6.022 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|-------|-------|------|--------|
| ATOM | 224 | CD | GLU A | 19138.972 | 8.446 | 6.592 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19138.749 | 8.429 | 7.820 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19138.435 | 9.259 | 5.810 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.458 | 5.260 | 4.107 | 1.00 | 0.00 H |
| ATOM | 228 | НА | GLU A | 19142.209 | 7.491 | 3.402 | 1.00 | 0.00 H |
| ATOM | 229 | IHB | GLU A | 19141.573 | 8.686 | 5.497 | 1.00 | 0.00 H |
| ATOM | 230 2 | 2HB | GLU A | 19140.288 | 8.623 | 4.298 | 1.00 | 0.00 H |
| ATOM | 231 | IHG | GLU A | 19139.378 | 6.637 | 5.558 | 1.00 | 0.00 H |
| ATOM | 232 2 | 2HG | GLU A | 19140.535 | 7.027 | 6.830 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.626 | 7.060 | 5.626 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VALA | 20144.644 | 6.514 | 6.516 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.014 | 5.893 | 7.757 | 1.00 | 0.00 C |
| ATOM | 236 | Ο | VAL A | 20143.157 | 6.499 | 8.401 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VALA | 20145.649 | 7.598 | 6.952 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VALĀ | 20146.811 | 6.976 | 7.710 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VALA | 20146.147 | 8.381 | 5.747 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20143.645 | 8.015 | 5.406 | 1.00 | 0.00 H |
| ATOM | 241 | HA | VAL A | 20145.184 | 5.750 | 5.976 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.142 | 8.284 | 7.615 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VALA | 20147.087 | 6.042 | 7.244 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20146.517 | 6.793 | 8.733 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20147.655 | 7.650 | 7.693 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20147.116 | 8.803 | 5.967 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20145.451 | 9.175 | 5.521 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VAL A | 20146.227 | 7.720 | 4.897 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.445 | 4.680 | 8.089 | 1.00 | 0.00 N |

| ATOM | 250 | CA | GLY A | 21143.912 | 3.996 | 9.253 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|-------|------|--------|
| ATOM | 251 | C | GLY A | 21142.916 | 2.914 | 8.885 | 1.00 | 0.00 C |
| ATOM | 252 | O | GLY A | 21142.848 | 1.876 | 9.542 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.130 | 4.247 | 7.539 | 1.00 | 0.00 H |
| ATOM | 254 1 | НА | GLY A | 21144.730 | 3.548 | 9.799 | 1.00 | 0.00 H |
| ATOM | 255 2 | 2HA | GLY A | 21143.424 | 4.720 | 9.888 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.142 | 3.158 | 7.834 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.145 | 2.196 | 7.379 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.791 | 1.093 | 6.546 | 1.00 | 0.00 C |
| ATOM | 259 | O | SER A | 22142.817 | 1.309 | 5.902 | 1.00 | 0.00 O |
| ATOM | 260 | CB | SER A | 22140.061 | 2.901 | 6.561 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22139.134 | 3.563 | 7.404 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.245 | 4.005 | 7.350 | 1.00 | 0.00 H |
| ATOM | 263 | HA | SER A | 22140.691 | 1.752 | 8.253 | 1.00 | 0.00 H |
| ATOM | 264 | IHB | SER A | 22140.522 | 3.631 | 5.911 | 1.00 | 0.00 H |
| ATOM | 265 2 | 2HB | SER A | 22139.532 | 2.172 | 5.965 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22139.608 | 4.049 | 8.083 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.182 | -0.088 | 6.563 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.698 | -1.224 | 5.809 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.307 | -1.125 | 4.338 | 1.00 | 0.00 C |
| ATOM | 270 | O | LEU A | 23140.274 | -0.549 | 3.998 | 1.00 | 0.00 O |
| ATOM | 271 | СВ | LEU A | 23141.177 | -2.535 | 6.399 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23141.354 | -2.680 | 7.911 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23140.277 | -3.584 | 8.491 | 1.00 | 0.00 C |
| ATOM | 274 | CD2 | LEU A | 23142.738 | -3.221 | 8.235 | 1.00 | 0.00 C |
| ATOM | 275 | Н | LEU A | 23140.367 | -0.198 | 7.095 | 1.00 | 0.00 H |
| ATOM | 276 | НА | LEU A | 23142.775 | -1.210 | 5.884 | 1.00 | 0.00 H |

| ATOM | 277 1 | IНВ | LEU A | 23140.123 | -2.612 | 6.172 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 278 2 | 2HB | LEU A | 23141.693 | -3.352 | 5.919 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23141.257 | -1.708 | 8.373 | 1.00 | 0.00 H |
| ATOM | 280 | IHD1 | LEU A | 23140.028 | -3.253 | 9.489 | 1.00 | 0.00 H |
| ATOM | 281 2 | 2HD1 | LEU A | 23140.642 | -4.600 | 8.529 | 1.00 | 0.00 H |
| ATOM | 282 3 | 3HD1 | LEU A | 23139.396 | -3.540 | 7.868 | 1.00 | 0.00 H |
| ATOM | 283 | HD2 | LEU A | 23143.421 | -2.963 | 7.439 | 1.00 | 0.00 H |
| ATOM | 284 2 | 2HD2 | LEU A | 23142.691 | -4.296 | 8.333 | 1.00 | 0.00 H |
| ATOM | 285 3 | 3HD2 | LEU A | 23143.085 | -2.791 | 9.162 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.140 | -1.689 | 3.470 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.882 | -1.663 | 2.035 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.477 | -2.887 | 1.349 | 1.00 | 0.00 C |
| ATOM | 289 | O | ALA A | 24143.416 | -3.502 | 1.856 | 1.00 | 0.00 O |
| ATOM | 290 | CB | ALA A | 24142.439 | -0.388 | 1.421 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.948 | -2.133 | 3.802 | 1.00 | 0.00 H |
| ATOM | 292 | HA | ALA A | 24140.811 | -1.667 | 1.890 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALA A | 24143.407 | -0.591 | 0.986 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24142.541 | 0.365 | 2.188 | 1.00 | 0.00 H |
| ATOM | 295 | 3HB | ALA A | 24141.767 | -0.034 | 0.654 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.926 | -3.237 | 0.191 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.403 | -4.388 | -0.566 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.632 | -4.020 | -2.029 | 1.00 | 0.00 C |
| ATOM | 299 | О | GLU A | 25141.891 | -3.223 | -2.602 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLUA | 25141.401 | -5.540 | -0.470 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25142.005 | -6.899 | -0.780 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25141.078 | -7.776 | -1.599 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25141.583 | -8.664 | -2.319 | 1.00 | 0.00 O |

| ATOM | 304 OE2 GLU A | 25139.847 | -7.577 | -1.520 | 1.00 | 0.00 O |
|--------|----------------|-----------|--------|----------------|------|--------|
| ATOM | 305 H GLUA | 25141.181 | -2.708 | -0.163 | 1.00 | 0.00 H |
| ATOM | 306 HA GLUA | 25143.341 | -4.703 | -0.135 | 1.00 | 0.00 H |
| ATOM | 307 1HB GLU A | 25140.998 | -5.569 | 0.532 | 1.00 | 0.00 H |
| ATOM | 308 2HB GLU A | 25140.596 | -5.360 | -1.167 | 1.00 | 0.00 H |
| ATOM . | 309 1HG GLU A | 25142.920 | -6.755 | -1.332 | 1.00 | 0.00 H |
| ATOM | 310 2HG GLU A | 25142.223 | -7.402 | 0.152 | 1.00 | 0.00 H |
| ATOM | 311 N VAL A | 26143.664 | -4.607 | -2.627 | 1.00 | 0.00 N |
| ATOM | 312 CA VALA | 26143.992 | -4.340 | -4.022 | 1.00 | 0.00 C |
| ATOM | 313 C VALA | 26143.563 | -5.497 | -4.918 | 1.00 | 0.00 C |
| ATOM | 314 O VAL A | 26143.381 | -6.622 | -4.450 | 1.00 | 0.00 O |
| ATOM | 315 CB VALA | 26145.500 | -4.093 | -4.208 | 1.00 | 0.00 C |
| ATOM | 316 CG1 VAL A | 26145.793 | -3.607 | -5.619 | 1.00 | 0.00 C |
| ATOM | 317 CG2 VAL A | 26146.010 | -3.097 | -3.177 | 1:00 | 0.00 C |
| ATOM | 318 H VALA | 26144.220 | -5.233 | -2.117 | 1.00 | 0.00 H |
| ATOM | 319 HA VALA | 26143.462 | -3.448 | -4.325 | 1.00 | 0.00 H |
| ATOM | 320 HB VALA | 26146.019 | -5.029 | -4.060 | 1.00 | 0.00 H |
| ATOM | 321 1HG1 VAL A | 26145.913 | -4.456 | -6.276 | 1.00 | 0.00 H |
| ATOM | 322 2HG1 VAL A | 26146.700 | -3.022 | -5.618 | 1.00 | 0.00 H |
| ATOM | 323 3HG1 VAL A | 26144.972 | -2.997 | -5.968 | 1.00 | 0.00 H |
| ATOM | 324 1HG2 VAL A | 26146.053 | -3.572 | -2.209 | 1.00 | 0.00 H |
| ATOM . | 325 2HG2 VAL A | 26145.341 | -2.250 | -3.133 | 1.00 | 0.00 H |
| ATOM | 326 3HG2 VAL A | 26146.998 | -2.762 | -3.457 | 1.00 | 0.00 H |
| ATOM | 327 N LYS A | 27143.402 | -5.215 | -6.206 | 1.00 | 0.00 N |
| ATOM | 328 CA LYSA | 27142.994 | -6.233 | - 7.167 | 1.00 | 0.00 C |
| ATOM | 329 C LYS A | 27144.201 | -6.795 | -7.911 | 1.00 | 0.00 C |
| ATOM | 330 O LYS A | 27144.125 | -7.090 | -9.103 | 1.00 | 0.00 O |

| ATOM | 331 | CB | LYS A | 27141.991 | -5.650 | -8.164 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|-----------|----------------|------|--------|
| ATOM | 332 | CG | LYSA | 27142.567 | -4.539 | -9.028 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27141.949 | -4.536 - | 10.418 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27142.791 | -5.328 -1 | 1.406 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27141.989 | -6.363 - | 12.115 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27143.561 | -4.300 | -6.518 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27142.519 | -7.033 | -6.620 | 1.00 | 0.00 H |
| ATOM | 338 1 | НВ | LYS A | 27141.647 | -6.440 | -8.815 | 1.00 | 0.00 H |
| ATOM | 339 2 | НВ | LYS A | 27141.149 | -5.252 | -7.619 | 1.00 | 0.00 H |
| ATOM | 340 1 | HG | LYS A | 27142.369 | -3.589 | -8.556 | 1.00 | 0.00 H |
| ATOM | 341 2 | HG | LYS A | 27143.634 | -4.683 | -9.117 | 1.00 | 0.00 H |
| ATOM | 342 1 | HD | LYS A | 27140.966 | -4.979 -1 | 0.364 | 1.00 | 0.00 H |
| ATOM | 343 2 | HD | LYS A | 27141.868 | -3.516 -1 | 0.762 | 1.00 | 0.00 H |
| ATOM | 344 1 | HE | LYS A | 27143.204 | -4.646 -1 | 2.134 | 1.00 | 0.00 H |
| ATOM | 345 2 | HE | LYS A | 27143.595 | -5.812 -1 | 0.871 | 1.00 | 0.00 H |
| ATOM | 346 1 | HZ | LYS A | 27142.045 | -7.269 -1 | 1.606 | 1.00 | 0.00 H |
| ATOM | 347 2 | HZ | LYS A | 27142.351 | -6.497 -1 | 3.081 | 1.00 | 0.00 H |
| ATOM | 348 3 | HZ | LYS A | 27140.993 | -6.068 -1 | 2.168 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28145.314 | -6.940 | -7.199 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28146.537 | -7.467 | - 7.793 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28146.479 | -8.988 | -7.899 | 1.00 | 0.00 C |
| ATOM | 352 | O | GLU A | 28145.509 | -9.614 | -7.472 | 1.00 | 0.00 O |
| ATOM | 353 | CB | GLU A | 28147.753 | -7.046 | -6.964 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28148.886 | -6.467 | - 7.797 | 1.00 | 0.00 C |
| ATOM | 355 | CD | GLU A | 28150.212 | -6.475 | -7.064 | 1.00 | 0.00 C |
| ATOM | 356 | OE1 | GLU A | 28150.759 | -5.379 | -6.815 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28150.704 | -7.575 | -6.738 | 1.00 | 0.00 O |

| ATOM | 358 | Н | GLU A | 28145.312 | - 6.687 | -6.252 | 1.00 | 0.00 H |
|------|--------------|------|-------|-------------|-----------|--------|------|--------|
| ATOM | 359 | НА | GLU A | 28146.628 | -7.052 | -8.786 | 1.00 | 0.00 H |
| ATOM | 360 1 | НВ | GLU A | 28147.445 | -6.299 | -6.248 | 1.00 | 0.00 H |
| ATOM | 361 2 | 2HB | GLU A | 28148.131 | -7.908 | -6.433 | 1.00 | 0.00 H |
| ATOM | 362 1 | HG | GLU A | 28148.987 | -7.052 | -8.699 | 1.00 | 0.00 H |
| ATOM | 363 2 | 2HG | GLU A | 28148.639 | -5.448 | -8.058 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29147.525 | -9.576 | -8.471 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29147.594 | -11.024 | -8.632 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29147.522 | -11.726 | -7.277 | 1.00 | 0.00 C |
| ATOM | 367 | O | ASN A | 29146.628 | -12.537 | -7.037 | 1.00 | 0.00 O |
| ATOM | 368 | CB | ASN A | 29148.882 | -11.416 | -9.358 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29148.671 | -11.604 - | 10.847 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29148.987 | -12.657 - | 11.403 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29148.135 | -10.581 - | 11.504 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29148.269 | -9.024 | -8.791 | 1.00 | 0.00 H |
| ATOM | 373 | HA | ASN A | 29146.747 | -11.331 | -9.228 | 1.00 | 0.00 H |
| ATOM | 374 1 | IНВ | ASN A | 29149.620 | -10.641 | -9.214 | 1.00 | 0.00 H |
| ATOM | 375 2 | 2HB | ASN A | 29149.253 | -12.343 | -8.946 | 1.00 | 0.00 H |
| ATOM | 376 | HD2 | ASN A | 29147.909 | -9.774 - | 10.996 | 1.00 | 0.00 H |
| ATOM | 377 2 | 2HD2 | ASN A | 29147.987 - | 10.675 -1 | 2.468 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30148.467 | -11.421 | -6.372 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30148.507 | -12.026 | -5.039 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30147.460 | -11.429 | -4.099 | 1.00 | 0.00 C |
| ATOM | 381 | O | PRO A | 30147.579 | -10.276 | -3.682 | 1.00 | 0.00 O |
| ATOM | 382 | СВ | PRO A | 30149.915 | -11.691 | -4.549 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30150.256 | -10.414 | -5.236 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30149.572 | -10.463 | -6.576 | 1.00 | 0.00 C |
| | | | | | | | | |

| ATOM | 385 | НА | PRO A | 30148.384 | -13.098 | -5.085 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 386 1 | НВ | PRO A | 30149.908 | -11.575 | -3.475 | 1.00 | 0.00 H |
| ATOM | 387 2 | 2HB | PRO A | 30150.595 | -12.482 | -4.827 | 1.00 | 0.00 H |
| ATOM | 388 1 | HG | PRO A | 30149.888 | -9.578 | -4.658 | 1.00 | 0.00 H |
| ATOM | 389 2 | 2HG | PRO A | 30151.326 | -10.340 | -5.363 | 1.00 | 0.00 H |
| ATOM | 390 1 | HD | PRO A | 30149.191 | -9.487 | -6.840 | 1.00 | 0.00 H |
| ATOM | 391 2 | 2HD | PRO A | 30150.254 | -10.817 | -7.334 | 1.00 | 0.00 H |
| ATOM | 392 | N | PRO A | 31146.417 | -12.204 | -3.751 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31145.353 | -11.735 | -2.857 | 1.00 | 0.00 C |
| ATOM | 394 | C | PRO A | 31145.844 | -11.540 | -1.426 | 1.00 | 0.00 C |
| ATOM | 395 | O | PRO A | 31145.741 | -12.443 | -0.595 | 1.00 | 0.00 O |
| ATOM | 396 | СВ | PRO A | 31144.313 | -12.857 | -2.917 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31145.088 | -14.071 | -3.297 | 1.00 | 0.00 C |
| ATOM | 398 | CD | PRO A | 31146.191 | -13.592 | -4.199 | 1.00 | 0.00 C |
| ATOM | 399 | НА | PRO A | 31144.914 | -10.815 | -3.213 | 1.00 | 0.00 H |
| ATOM | 400 1 | НВ | PRO A | 31143.847 | 12.973 | -1.949 | 1.00 | 0.00 H |
| ATOM | 401 2 | 2HB | PRO A | 31143.565 | 12.620 | -3.658 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31145.501 | -14.535 | -2.413 | 1.00 | 0.00 H |
| ATOM | 403 2 | 2HG | PRO A | 31144.449 | -14.766 | -3.823 | 1.00 | 0.00 H |
| ATOM | 404 | HD | PRO A | 31147.078 | -14.192 | -4.061 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31145.872 | -13.617 | -5.230 | 1.00 | 0.00 H |
| ATOM | 406 | N | PHE A | 32146.377 | -10.356 | -1.146 | 1.00 | 0.00 N |
| ATOM | 407 | CA | PHE A | 32146.885 | -10.041 | 0.185 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.947 | -9.083 | 0.912 | 1.00 | 0.00 C |
| ATOM | 409 | О | PHE A | 32144.998 | -8.562 | 0.324 | 1.00 | 0.00 O |
| ATOM | 410 | СВ | PHE A | 32148.283 | -9.430 | 0.090 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.404 | -8.366 | -0.964 | 1.00 | 0.00 C |

| ATOM | 412 | CD1 | PHE A | 32147.687 | -7.185 | -0.859 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 413 | | PHE A | 32149.233 | -8.548 | -2.059 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32147.796 | -6.205 | -1.827 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32149.346 | -7.572 | -3.030 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.626 | -6.397 | -2.914 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32146.430 | -9.677 | -1.850 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.941 | -10.963 | 0.744 | 1.00 | 0.00 H |
| ATOM | 419 1 | НВ | PHE A | 32148.540 | -8.987 | 1.040 | 1.00 | 0.00 H |
| ATOM | 420 2 | НВ | PHE A | 32148.994 - | -10.210 | -0.141 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32147.038 | -7.032 | -0.010 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32149.796 | -9.465 | -2.151 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32147.232 | -5.289 | -1.734 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32149.995 | -7.724 | -3.879 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.712 | -5.632 | -3.672 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.217 | -8.856 | 2.193 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.397 | -7.958 | 2.999 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.269 | -6.990 | 3.793 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.270 | -7.387 | 4.389 | 1.00 | 0.00 O |
| ATOM | 430 | CB | TYR A | 33144.511 | -8.763 | 3.952 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.249 | -9.290 | 3.306 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.903 | -10.632 | 3.406 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.405 | -8.447 | 2.595 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.751 | -11.118 | 2.817 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.251 | -8.925 | 2.003 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.929 | -10.261 | 2.116 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.781 | -10.740 | 1.529 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.987 | -9.300 | 2.605 | 1.00 | 0.00 H |

| ATOM | 439 | HA | TYR A | 33144.769 | -7.392 | 2.329 | 1.00 | 0.00 H |
|------|-----|------------|-------|-------------|---------|-------|------|--------|
| ATOM | 440 | 1HB | TYR A | 33145.069 | -9.608 | 4.325 | 1.00 | 0.00 H |
| ATOM | 441 | 2HB | TYR A | 33144.222 | -8.134 | 4.780 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33143.549 - | 11.302 | 3.956 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.661 | -7.401 | 2.507 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33141.500 - | 12.165 | 2.907 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.609 | -8.253 | 1.455 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33139.736 | -10.436 | 0.620 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.880 | -5.719 | 3.796 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.637 | -4.715 | 4.519 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34145.778 | -3.546 | 4.957 | 1.00 | 0.00 C |
| ATOM | 450 | О | GLY A | 34144.551 | -3.643 | 4.984 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.074 | -5.462 | 3.302 | 1.00 | 0.00 H |
| ATOM | 452 | 1HA | GLY A | 34147.077 | -5.172 | 5.393 | 1.00 | 0.00 H |
| ATOM | 453 | 2HA | GLY A | 34147.427 | -4.348 | 3.881 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.423 | -2.435 | 5.301 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VALA | 35145.710 | -1.242 | 5.740 | 1.00 | 0.00 C |
| ATOM | 456 | , C | VAL A | 35146.363 | 0.022 | 5.187 | 1.00 | 0.00 C |
| ATOM | 457 | O | VAL A | 35147.577 | 0.070 | 4.991 | 1.00 | 0.00 O |
| ATOM | 458 | СВ | VALA | 35145.657 | -1.154 | 7.279 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VALA | 35147.060 | -1.060 | 7.861 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35144.809 | 0.029 | 7.720 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.402 | -2.420 | 5.259 | 1.00 | 0.00 H |
| ATOM | 462 | HA | VAL A | 35144.698 | -1.304 | 5.370 | 1.00 | 0.00 H |
| ATOM | 463 | HB | VAL A | 35145.199 | -2.057 | 7.654 | 1.00 | 0.00 H |
| ATOM | 464 | 1HG1 | VAL A | 35147.690 | -1.812 | 7.406 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VAL A | 35147.020 | -1.222 | 8.927 | 1.00 | 0.00 H |

| ATOM | 466 3HG1 | VALA | 35147.468 | -0.080 | 7.660 | 1.00 | 0.00 H |
|------|----------|-------|-----------|--------|-------|------|--------|
| ATOM | 467 1HG2 | VALA | 35143.784 | -0.133 | 7.423 | 1.00 | 0.00 H |
| ATOM | 468 2HG2 | VAL A | 35145.180 | 0.932 | 7.257 | 1.00 | 0.00 H |
| ATOM | 469 3HG2 | VALA | 35144.861 | 0.129 | 8.795 | 1.00 | 0.00 H |
| ATOM | 470 N | ILE A | 36145.548 | 1.042 | 4.939 | 1.00 | 0.00 N |
| ATOM | 471 CA | ILE A | 36146.046 | 2.306 | 4.409 | 1.00 | 0.00 C |
| ATOM | 472 C | ILE A | 36146.970 | 2.992 | 5.410 | 1.00 | 0.00 C |
| ATOM | 473 O | ILE A | 36146.688 | 3.027 | 6.607 | 1.00 | 0.00 O |
| ATOM | 474 CB | ILE A | 36144.891 | 3.262 | 4.051 | 1.00 | 0.00 C |
| ATOM | 475 CG1 | ILE A | 36143.876 | 2.558 | 3.149 | 1.00 | 0.00 C |
| ATOM | 476 CG2 | ILE A | 36145.430 | 4.514 | 3.374 | 1.00 | 0.00 C |
| ATOM | 477 CD1 | ILE A | 36142.709 | 3.435 | 2.752 | 1.00 | 0.00 C |
| ATOM | 478 H | ILE A | 36144.590 | 0.943 | 5.117 | 1.00 | 0.00 H |
| ATOM | 479 HA | ILE A | 36146.603 | 2.093 | 3.508 | 1.00 | 0.00 H |
| ATOM | 480 HB | ILE A | 36144.404 | 3.561 | 4.967 | 1.00 | 0.00 H |
| ATOM | 481 1HG1 | ILE A | 36144.369 | 2.234 | 2.246 | 1.00 | 0.00 H |
| ATOM | 482 2HG1 | ILE A | 36143.482 | 1.695 | 3.667 | 1.00 | 0.00 H |
| ATOM | 483 1HG2 | ILE A | 36146.162 | 4.235 | 2.630 | 1.00 | 0.00 H |
| ATOM | 484 2HG2 | ILE A | 36145.893 | 5.152 | 4.112 | 1.00 | 0.00 H |
| ATOM | 485 3HG2 | ILE A | 36144.618 | 5.044 | 2.898 | 1.00 | 0.00 H |
| ATOM | 486 1HD1 | ILE A | 36142.535 | 3.343 | 1.690 | 1.00 | 0.00 H |
| ATOM | 487 2HD1 | ILE A | 36142.935 | 4.464 | 2.992 | 1.00 | 0.00 H |
| ATOM | 488 3HD1 | ILE A | 36141.826 | 3.126 | 3.290 | 1.00 | 0.00 H |
| ATOM | 489 N | ARG A | 37148.076 | 3.535 | 4.910 | 1.00 | 0.00 N |
| ATOM | 490 CA | ARG A | 37149.042 | 4.220 | 5.761 | 1.00 | 0.00 C |
| ATOM | 491 C | ARG A | 37149.240 | 5.664 | 5.308 | 1.00 | 0.00 C |
| ATOM | 492 O | ARG A | 37148.974 | 6.601 | 6.060 | 1.00 | 0.00 O |

| ATOM | 493 | СВ | ARG A | 37150.382 | 3.480 | 5.742 | 1.00 | 0.00 C |
|------|-------|-------|-------|-----------|-------|--------|------|--------|
| ATOM | 494 | CG | ARG A | 37150.258 | 1.992 | 6.024 | 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | 37149.607 | 1.733 | 7.373 | 1.00 | 0.00 C |
| ATOM | 496 | NE | ARG A | 37150.302 | 2.420 | 8.458 | 1.00 | 0.00 N |
| ATOM | 497 | CZ | ARG A | 37149.765 | 2.653 | 9.653 | 1.00 | 0.00 C |
| ATOM | 498 | NH1 | ARG A | 37148.527 | 2.255 | 9.921 | 1.00 | 0.00 N |
| ATOM | 499 | NH2 | ARG A | 37150.467 | 3.285 | 10.584 | 1.00 | 0.00 N |
| ATOM | 500 | Н | ARG A | 37148.246 | 3.474 | 3.947 | 1.00 | 0.00 H |
| ATOM | 501 | HA | ARG A | 37148.656 | 4.221 | 6.768 | 1.00 | 0.00 H |
| ATOM | 502 | lНВ | ARG A | 37150.835 | 3.605 | 4.769 | 1.00 | 0.00 H |
| ATOM | 503 2 | 2HB | ARG A | 37151.030 | 3.914 | 6.489 | 1.00 | 0.00 H |
| ATOM | 504 | IHG | ARG A | 37149.657 | 1.537 | 5.251 | 1.00 | 0.00 H |
| ATOM | 505 2 | 2HG | ARG A | 37151.245 | 1.553 | 6.020 | 1.00 | 0.00 H |
| ATOM | 506 | IHD | ARG A | 37148.585 | 2.079 | 7.337 | 1.00 | 0.00 H |
| ATOM | 507 2 | 2HD | ARG A | 37149.620 | 0.670 | 7.565 | 1.00 | 0.00 H |
| ATOM | 508 | HE | ARG A | 37151.219 | 2.724 | 8.288 | 1.00 | 0.00 H |
| ATOM | 509 | 1HH1. | ARG A | 37147.992 | 1.778 | 9.224 | 1.00 | 0.00 H |
| ATOM | 510 2 | 2HH1. | ARG A | 37148.129 | 2.432 | 10.820 | 1.00 | 0.00 H |
| ATOM | 511 | HH2 | ARG A | 37151.400 | 3.585 | 10.387 | 1.00 | 0.00 H |
| ATOM | 512 2 | 2HH2 | ARG A | 37150.063 | 3.460 | 11.482 | 1.00 | 0.00 H |
| ATOM | 513 | N | TRPA | 38149.705 | 5.835 | 4.075 | 1.00 | 0.00 N |
| ATOM | 514 | CA | TRP A | 38149.938 | 7.166 | 3.525 | 1.00 | 0.00 C |
| ATOM | 515 | C | TRPA | 38149.254 | 7.323 | 2.169 | 1.00 | 0.00 C |
| ATOM | 516 | О | TRPA | 38149.360 | 6.454 | 1.304 | 1.00 | 0.00 O |
| ATOM | 517 | CB | TRP A | 38151.441 | 7.431 | 3.388 | 1.00 | 0.00 C |
| ATOM | 518 | CG | TRPA | 38151.763 | 8.666 | 2.600 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRPA | 38151.926 | 9.931 | 3.086 | 1.00 | 0.00 C |

| ATOM | 520 | CD2 | TRP A | 38151.955 | 8.752 | 1.183 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 521 | NE1 | TRPA | 38152.207 | 10.799 | 2.058 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRPA | 38152.231 | 10.098 | 0.880 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38151.921 | 7.821 | 0.141 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRPA | 38152.471 | 10.535 | -0.422 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.159 | 8.254 | -1.149 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRPA | 38152.431 | 9.601 | -1.420 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRPA | 38149.898 | 5.049 | 3.523 | 1.00 | 0.00 H |
| ATOM | 528 | НА | TRPA | 38149.516 | 7.885 | 4.211 | 1.00 | 0.00 H |
| ATOM | 529 | 1HB | TRPA | 38151.871 | 7.544 | 4.373 | 1.00 | 0.00 H |
| ATOM | 530 2 | 2HB | TRPA | 38151.904 | 6.589 | 2.894 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38151.842 | 10.198 | 4.129 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38152.366 | 11.761 | 2.153 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRPA | 38151.713 | 6.779 | 0.331 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38152.679 | 11.570 | -0.648 | 1.00 | 0.00 H |
| ATOM | 535 | HZ3 | TRPA | 38152.138 | 7.548 | -1.966 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRP A | 38152.612 | 9.895 | -2.444 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.559 | 8.442 | 1.993 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39147.864 | 8.725 | 0.744 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILE A | 39148.314 | 10.064 | 0.170 | 1.00 | 0.00 C |
| ATOM | 540 | О | ILE A | 39147.947 | 11.122 | 0.681 | 1.00 | 0.00 O |
| ATOM | 541 | СВ | ILE A | 39146.337 | 8.750 | 0.942 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39145.876 | 7.502 | 1.698 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.630 | 8.855 | -0.400 | 1.00 | 0.00 C |
| ATOM | 544 | CD1 | ILE A | 39144.499 | 7.639 | 2.309 | 1.00 | 0.00 C |
| ATOM | 545 | Н | ILE A | 39148.519 | 9.097 | 2.721 | 1.00 | 0.00 H |
| ATOM | 546 | HA | ILE A | 39148.104 | 7.941 | 0.041 | 1.00 | 0.00 H |

| ATOM | 547 | HB | ILE A | 39146.085 | 9.626 | 1.522 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 548 | 1HG1 | ILE A | 39145.854 | 6.665 | 1.016 | 1.00 | 0.00 H |
| ATOM | 549 2 | 2HG1 | ILE A | 39146.575 | 7.294 | 2.494 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39146.098 | 9.626 | -0.994 | 1.00 | 0.00 H |
| ATOM | 551 2 | 2HG2 | ILE A | 39144.590 | 9.104 | -0.243 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39145.699 | 7.909 | -0.918 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.001 | 8.499 | 1.886 | 1.00 | 0.00 H |
| ATOM | 554 2 | 2HD1 | ILE A | 39144.590 | 7.764 | 3.378 | 1.00 | 0.00 H |
| ATOM | 555 3 | 3HD1 | ILE A | 39143.922 | 6.750 | 2.099 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.115 | 10.011 | -0.889 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.604 | 11.231 | -1.504 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.212 | 10.994 | -2.873 | 1.00 | 0.00 C |
| ATOM | 559 | O | GLY A | 40150.068 | 9.916 | -3.447 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.379 | 9.141 | -1.252 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40148.785 | 11.925 | -1.603 | 1.00 | 0.00 H |
| ATOM | 562 2 | 2HA | GLY A | 40150.353 | 11.667 | -0.862 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41150.892 | 12.010 | -3.394 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.525 | 11.919 | -4.703 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41153.000 | 12.311 | -4.618 | 1.00 | 0.00 C |
| ATOM | 566 | O | GLN A | 41153.325 | 13.461 | -4.321 | 1.00 | 0.00 O |
| ATOM | 567 | CB | GLN A | 41150.799 | 12.825 | -5.696 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | 41149.288 | 12.653 | -5.685 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.551 | 13.969 | -5.825 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.474 | 14.755 | -4.881 | 1.00 | 0.00 O |
| ATOM | 571 | NE2 | GLN A | 41148.004 | 14.216 | -7.009 | 1.00 | 0.00 N |
| ATOM | 572 | Н | GLN A | 41150.968 | 12.844 | -2.886 | 1.00 | 0.00 H |
| ATOM | 573 | HA | GLN A | 41151.451 | 10.897 | -5.040 | 1.00 | 0.00 H |

| ATOM | 574 | 1HB | GLN A | 41151.023 | 13.853 | -5.456 | 1.00 | 0.00 H |
|--------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 575 | 2HB | GLN A | 41151.158 | 12.610 | -6.690 | 1.00 | 0.00 H |
| ATOM | 576 | 1HG | GLN A | 41149.005 | 12.010 | -6.504 | 1.00 | 0.00 H |
| ATOM | 577 | 2HG | GLN A | 41148.999 | 12.192 | -4.752 | 1.00 | 0.00 H |
| ATOM | 578 | 1HE2 | GLN A | 41148.106 | 13.544 | -7.715 | 1.00 | 0.00 H |
| ATOM | 579 | 2HE2 | GLN A | 41147.522 | 15.061 | -7.130 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42153.917 | 11.361 | -4.876 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.360 | 11.623 | -4.822 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.779 | 12.746 | -5.766 | 1.00 | 0.00 C |
| ATOM | 583 | O | PRO A | 42155.066 | 13.071 | -6.715 | 1.00 | 0.00 O |
| ATOM | 584 | СВ | PRO A | 42155.986 | 10.295 | -5.261 | 1.00 | 0.00 C |
| ATOM | 585 | CG | PRO A | 42154.937 | 9.272 | -5.000 | 1.00 | 0.00 C |
| ATOM | 586 | CD | PRO A | 42153.626 | 9.962 | -5.237 | 1.00 | 0.00 C |
| ATOM | 587 | НА | PRO A | 42155.680 | 11.861 | -3.819 | 1.00 | 0.00 H |
| ATOM - | 588 | 1HB | PRO A | 42156.239 | 10.344 | -6.311 | 1.00 | 0.00 H |
| ATOM | 589 2 | 2HB | PRO A | 42156.877 | 10.105 | -4.680 | 1.00 | 0.00 H |
| ATOM | 590 | 1HG | PRO A | 42155.053 | 8.442 | -5.681 | 1.00 | 0.00 H |
| ATOM | 5912 | 2HG | PRO A | 42155.002 | 8.931 | -3.976 | 1.00 | 0.00 H |
| ATOM | 592 | 1HD | PRO A | 42153.340 | 9.882 | -6.276 | 1.00 | 0.00 H |
| ATOM | 593 2 | 2HD | PRO A | 42152.859 | 9.550 | -4.598 | 1.00 | 0.00 H |
| ATOM | 594 | N | PRO A | 43156.951 | 13.355 | -5.515 | 1.00 | 0.00 N |
| ATOM | 595 | CA | PRO A | 43157.466 | 14.446 | -6.347 | 1.00 | 0.00 C |
| ATOM | 596 | C | PRO A | 43157.941 | 13.958 | -7.711 | 1.00 | 0.00 C |
| ATOM | 597 | O | PRO A | 43159.115 | 13.636 | -7.891 | 1.00 | 0.00 O |
| ATOM | 598 | CB | PRO A | 43158:643 | 14.986 | -5.535 | 1.00 | 0.00 C |
| ATOM | 599 | CG | PRO A | 43159.098 | 13.830 | -4.714 | 1.00 | 0.00 C |
| ATOM | 600 | CD | PRO A | 43157.863 | 13.027 | -4.403 | 1.00 | 0.00 C |

| ATOM | 601 | HA | PRO A | 43156.729 | 15.225 | -6.481 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|----------|--------|------|----------|
| ATOM | 602 1 | НВ | PRO A | 43159.419 | 15.323 | -6.207 | 1.00 | 0.00 H |
| ATOM | 603 2 | HB | PRO A | 43158.312 | 15.805 | -4.915 | 1.00 | 0.00 H |
| ATOM | 604 1 | HG | PRO A | 43159.800 | 13.233 | -5.277 | 1.00 | 0.00 H |
| ATOM | 605 2 | HG | PRO A | 43159.553 | 14.185 | -3.800 | 1.00 | 0.00 H |
| ATOM | 606 1 | HD | PRO A | 43158.092 | 11.973 | -4.391 | 1.00 | 0.00 H |
| ATOM | 607 2 | 2HD | PRO A | 43157.442 | 13.334 | -3.457 | 1.00 | 0.00 H |
| ATOM | 608 | N | GLY A | 44157.022 | 13.906 | -8.667 | 1.00 | 0.00 N |
| ATOM | 609 | CA | GLY A | 44157.369 | 13.457 - | 10.002 | 1.00 | 0.00 C |
| ATOM | 610 | C | GLY A | 44156.170 | 12.942 - | 10.771 | 1.00 | 0.00 C |
| ATOM | 611 | O | GLY A | 44155.925 | 13.359 - | 11.903 | 1.00 | 0.00 O |
| ATOM | 612 | Н | GLY A | 44156.101 | 14.175 | -8.467 | 1.00 | 0.00 H |
| ATOM | 613 1 | HA | GLY A | 44157.804 | 14.281 - | 10.546 | 1.00 | 0.00 H · |
| ATOM | 614 2 | 2HA | GLY A | 44158.100 | 12.664 | -9.924 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45155.420 | 12.034 - | 10.156 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEÚ A | 45154.240 | 11.463 - | 10.793 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45152.994 | 11.726 | -9.956 | 1.00 | 0.00 C |
| ATOM | 618 | O | LEU A | 45152.847 | 11.184 | -8.860 | 1.00 | 0.00 O |
| ATOM | 619 | CB | LEU A | 45154.422 | 9.959 - | 10.999 | 1.00 | 0.00 C |
| ATOM | 620 | CG | LEU A | 45154.906 | 9.191 | -9.766 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.533 | 7.718 | -9.873 | 1.00 | 0.00 C |
| ATOM | 622 | CD2 | LEU A | 45156.411 | 9.354 | -9.592 | 1.00 | 0.00 C |
| ATOM | 623 | Н | LEU A | 45155.664 | 11.743 | -9.251 | 1.00 | 0.00 H |
| ATOM | 624 | HA | LEU A | 45154.119 | 11.938 - | 11.754 | 1.00 | 0.00 H |
| ATOM | 625 1 | HB | LEU A | 45153.476 | 9.542 - | 11.310 | 1.00 | 0.00 H |
| ATOM | 626 2 | ΣHB | LEU A | 45155.140 | 9.810 - | 11.791 | 1.00 | 0.00 H |
| ATOM | 627 | HG | LEU A | 45154.421 | 9.594 | -8.889 | 1.00 | 0.00 H |

| ATOM | 628 1 | HD1 | LEU A | 45155.414 | 7.111 | -9.728 | 1.00 | 0.00 H | |
|------|-------|-----|-------|-----------|----------|---------|------|--------|--|
| ATOM | 629 2 | HD1 | LEU A | 45154.117 | 7.521 - | 10.849 | 1.00 | 0.00 H | |
| ATOM | 630 3 | HD1 | LEU A | 45153.803 | 7.477 | -9.114 | 1.00 | 0.00 H | |
| ATOM | 631 1 | HD2 | LEU A | 45156.770 | 10.126 - | 10.257 | 1.00 | 0.00 H | |
| ATOM | 632 2 | HD2 | LEU A | 45156.904 | 8.422 | -9.824 | 1.00 | 0.00 H | |
| ATOM | 633 3 | HD2 | LEU A | 45156.626 | 9.631 | -8.571 | 1.00 | 0.00 H | |
| ATOM | 634 | N | ASN A | 46152.096 | 12.558 | -10.474 | 1.00 | 0.00 N | |
| ATOM | 635 | CA | ASN A | 46150.868 | 12.879 | -9.761 | 1.00 | 0.00 C | |
| ATOM | 636 | C | ASN A | 46149.905 | 11.697 | -9.796 | 1.00 | 0.00 C | |
| ATOM | 637 | O | ASN A | 46149.319 | 11.390 | -10.834 | 1.00 | 0.00 O | |
| ATOM | 638 | СВ | ASN A | 46150.205 | 14.113 | -10.378 | 1.00 | 0.00 C | |
| ATOM | 639 | CG | ASN A | 46149.419 | 14.917 | -9.361 | 1.00 | 0.00 C | |
| ATOM | 640 | OD1 | ASN A | 46148.199 | 15.047 | -9.464 | 1.00 | 0.00 O | |
| ATOM | 641 | ND2 | ASN A | 46150.117 | 15.463 | -8.372 | 1.00 | 0.00 N | |
| ATOM | 642 | Н | ASN A | 46152.264 | 12.961 | -11.350 | 1.00 | 0.00 H | |
| ATOM | 643 | НА | ASN A | 46151.123 | 13.092 | -8.733 | 1.00 | 0.00 H | |
| ATOM | 644 1 | HB | ASN A | 46150.967 | 14.749 | -10.800 | 1.00 | 0.00 H | |
| ATOM | 645 2 | :HB | ASN A | 46149.530 | 13.797 | -11.160 | 1.00 | 0.00 H | |
| ATOM | 646 1 | HD2 | ASN A | 46151.086 | 15.318 | -8.353 | 1.00 | 0.00 H | |
| ATOM | 647 2 | HD2 | ASN A | 46149.634 | 15.989 | -7.700 | 1.00 | 0.00 H | |
| ATOM | 648 | N | GLU A | 47149.747 | 11.040 | -8.654 | 1.00 | 0.00 N | |
| ATOM | 649 | CA | GLU A | 47148.857 | 9.891 | -8.546 | 1.00 | 0.00 C | |
| ATOM | 650 | C | GLU A | 47148.612 | 9.532 | -7.084 | 1.00 | 0.00 C | |
| ATOM | 651 | O | GLU A | 47149.551 | 9.232 | -6.346 | 1.00 | 0.00 O | |
| ATOM | 652 | CB | GLU A | 47149.445 | 8.687 | -9.288 | 1.00 | 0.00 C | |
| ATOM | 653 | CG | GLU A | 47150.953 | 8.556 | -9.150 | 1.00 | 0.00 C | |
| ATOM | 654 | CD | GLU A | 47151.556 | 7.633 | -10.192 | 1.00 | 0.00 C | |

| ATOM | 655 | OE1 | GLU A | 47151.850 | 6.467 | -9.853 | 1.00 | 0.00 O |
|------|-----|--------------|-------|-----------|---------|---------|--------|--------|
| ATOM | 656 | OE2 | GLU A | 47151.731 | 8.076 - | 11.347 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47150.243 | 11.335 | -7.862 | 1.00 | 0.00 H |
| ATOM | 658 | HA | GLU A | 47147.916 | 10.158 | -9.000 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.991 | 7.786 | -8.902 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47149.208 | 8.776 | -10.338 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47151.398 | 9.534 | -9.258 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47151.182 | 8.166 | -8.169 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.351 | 9.557 | -6.671 | 1.00 \ | 0.00 N |
| ATOM | 664 | CA | VAL A | 48146.997 | 9.226 | -5.298 | 1.00 | 0.00 C |
| ATOM | 665 | C | VALA | 48147.343 | 7.775 | -4.989 | 1.00 | 0.00 C |
| ATOM | 666 | Ο | VAL A | 48146.591 | 6.861 | -5.329 | 1.00 | 0.00 O |
| ATOM | 667 | CB | VALA | 48145.499 | 9.456 | -5.029 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VALA | 48145.192 | 9.299 | -3.547 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VALA | 48145.072 | 10.828 | -5.527 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.643 | 9.799 | -7.304 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.567 | 9.869 | -4.641 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48144.938 | 8.708 | -5.570 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VAL A | 48144.163 | 9.571 | -3.362 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VAL A | 48145.843 | 9.943 | -2.974 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VALA | 48145.351 | 8.273 | -3.252 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48144.130 | 11.099 | -5.073 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VAL A | 48144.958 | 10.801 | -6.601 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VALA | 48145.822 | 11.558 | -5.263 | 1.00 | 0.00 H |
| ATOM | 679 | N | LEU A | 49148.487 | 7.569 | -4.345 | 1.00 | 0.00 N |
| ATOM | 680 | CA | LEU A | 49148.934 | 6.227 | -3.994 | 1.00 | 0.00 C |
| ATOM | 681 | \mathbf{C} | LEU A | 49148.788 | 5.983 | -2.498 | 1.00 | 0.00 C |

| ATOM | 682 | Ο | LEU A | 49149.449 | 6.633 | -1.687 | 1.00 | 0.00 O |
|--------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 683 | СВ | LEU A | 49150.390 | 6.023 | -4.417 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.667 | 6.237 | -5.906 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49152.113 | 6.656 | -6.125 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEU A | 49150.352 | 4.974 | -6.693 | 1.00 | 0.00 C |
| ATOM | 687 | Н | LEU A | 49149.045 | 8.336 | -4.102 | 1.00 | 0.00 H |
| ATOM | 688 | HA | LEU A | 49148.313 | 5.521 | -4.524 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49151.005 | 6.711 | -3.855 | 1.00 | 0.00 H |
| ATOM | 690 | 2HB | LEU A | 49150.680 | 5.015 | -4.162 | 1.00 | 0.00 H |
| ATOM | 691 | HG | LEU A | 49150.032 | 7.029 | -6.275 | 1.00 | 0.00 H |
| ATOM | 692 | 1HD1 | LEU A | 49152.177 | 7.734 | -6.140 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49152.464 | 6.261 | -7.067 | 1.00 | 0.00 H |
| ATOM | 694 | 3HD1 | LEU A | 49152.725 | 6.271 | -5.323 | 1.00 | 0.00 H |
| ATOM | 695 | 1HD2 | LEU A | 49151.242 | 4.367 | -6.770 | 1.00 | 0.00 H |
| ATOM | 696 | 2HD2 | LEU A | 49150.012 | 5.241 | -7.682 | 1.00 | 0.00 H |
| ATOM | 697 | 3HD2 | LEU A | 49149.579 | 4.416 | -6.185 | 1.00 | 0.00 H |
| ATOM | 698 | N | ALA A | 50147.919 | 5.047 | -2.139 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.689 | 4.724 | -0.738 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALA A | 50148.600 | 3.591 | -0.281 | 1.00 | 0.00 C |
| ATOM | 701 | О | ALA A | 50148.489 | 2.461 | -0.758 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.230 | 4.357 | -0.514 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.421 | 4.564 | -2.831 | 1.00 | 0.00 H |
| ATOM | 704 | НА | ALA A | 50147.909 | 5.608 | -0.156 | 1.00 | 0.00 H |
| ATOM | 705 | 1HB | ALA A | 50145.901 | 4.754 | 0.435 | 1.00 | 0.00 H |
| ATOM - | 706 | 2HB | ALA A | 50146.126 | 3.282 | -0.509 | 1.00 | 0.00 H |
| ATOM | 707 | 3HB | ALA A | 50145.628 | 4.775 | -1.307 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.502 | 3.899 | 0.645 | 1.00 | 0.00 N |

| ATOM | 709 | CA | GLY A | 51150.420 | 2.895 | 1.151 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 710 | C | GLY A | 51149.722 | 1.838 | 1.983 | 1.00 | 0.00 C |
| ATOM | 711 | Ο | GLY A | 51149.241 | 2.120 | 3.081 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.545 | 4.816 | 0.988 | 1.00 | 0.00 H |
| ATOM | 713 | 1HA | GLY A | 51150.907 | 2.415 | 0.315 | 1.00 | 0.00 H |
| ATOM | 714 | 2HA | GLY A | 51151.168 | 3.381 | 1.759 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.667 | 0.617 | 1.461 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.023 | -0.486 | 2.164 | 1.00 | 0.00 C |
| ATOM | 717 | С | LEU A | 52150.052 | -1.340 | 2.897 | 1.00 | 0.00 C |
| ATOM | 718 | О | LEU A | 52151.062 | -1.744 | 2.320 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.231 | -1.352 | 1.183 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52146.974 | -0.695 | 0.609 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.452 | -1.490 | -0.579 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52145.903 | -0.569 | 1.680 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.068 | 0.453 | 0.582 | 1.00 | 0.00 H |
| ATOM | 724 | НА | LEU A | 52148.342 | -0.064 | 2.889 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.882 | -1.616 | 0.362 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52147.935 | -2.258 | 1.692 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.222 | 0.298 | 0.262 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52145.685 | -2.174 | -0.246 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52147.263 | -2.047 | -1.023 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52146.037 | -0.812 | -1.311 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52145.344 | 0.343 | 1.526 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52146.368 | -0.544 | 2.655 | 1.00 | 0.00 H |
| ATOM | 733 | 3HD2 | LEU A | 52145.234 | -1.414 | 1.622 | 1.00 | 0.00 H |
| ATOM | 734 | N | GLU A | 53149.790 | -1.612 | 4.171 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.694 | -2.418 | 4.983 | 1.00 | 0.00 C |

| ATOM | 736 | C | GLU A | 53150.200 | -3.859 | 5.076 | 1.00 | 0.00 C |
|------|--------------|------|-------|-----------|---------|-------|------|--------|
| ATOM | 737 | О | GLU A | 53149.205 | -4.142 | 5.744 | 1.00 | 0.00 O |
| ATOM | 738 | СВ | GLU A | 53150.826 | -1.819 | 6.384 | 1.00 | 0.00 C |
| ATOM | 739 | CG | GLU A | 53151.783 | -2.584 | 7.284 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.317 | -2.629 | 8.726 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53151.200 | -1.550 | 9.345 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53151.071 | - 3.742 | 9.236 | 1.00 | 0.00 O |
| ATOM | 743 | Н | GLU A | 53148.969 | -1.262 | 4.575 | 1.00 | 0.00 H |
| ATOM | 744 | НА | GLU A | 53151.662 | -2.413 | 4.505 | 1.00 | 0.00 H |
| ATOM | 745 | HB | GLU A | 53151.182 | -0.804 | 6.297 | 1.00 | 0.00 H |
| ATOM | 746 2 | 2HB | GLU A | 53149.854 | -1.812 | 6.853 | 1.00 | 0.00 H |
| ATOM | 747 1 | HG | GLU A | 53151.870 | -3.597 | 6.919 | 1.00 | 0.00 H |
| ATOM | 748 2 | 2HG | GLU A | 53152.751 | -2.105 | 7.248 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54150.903 | -4.765 | 4.405 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.537 | -6.176 | 4.412 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54150.705 | -6.775 | 5.805 | 1.00 | 0.00 C |
| ATOM | 752 | O | LEU A | 54151.577 | -6.360 | 6.568 | 1.00 | 0.00 O |
| ATOM | 753 | СВ | LEU A | 54151.389 | -6.950 | 3.404 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.447 | -6.342 | 2.002 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.766 | -6.680 | 1.327 | 1.00 | 0.00 C |
| ATOM | 756 | .CD2 | LEU A | 54150.276 | -6.829 | 1.162 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.686 | -4.477 | 3.891 | 1.00 | 0.00 H |
| ATOM | 758 | НА | LEU A | 54149.498 | -6.250 | 4.124 | 1.00 | 0.00 H |
| ATOM | 759 | HB | LEU A | 54152.396 | -7.013 | 3.790 | 1.00 | 0.00 H |
| ATOM | 760 2 | 2HB | LEU A | 54150.990 | -7.951 | 3.321 | 1.00 | 0.00 H |
| ATOM | 761 | HG | LEU A | 54151.378 | -5.266 | 2.081 | 1.00 | 0.00 H |
| ATOM | 762 | HD1 | LEU A | 54153.136 | -7.620 | 1.710 | 1.00 | 0.00 H |

| ATOM | 763 2 | 2HD1 | LEU A | 54153.485 | -5.901 | 1.531 | 1.00 | 0.00 H |
|------|-------|------|-------|-------------|---------|-------|------|--------|
| ATOM | 764 | 3HD1 | LEU A | 54152.615 | -6.761 | 0.261 | 1.00 | 0.00 H |
| ATOM | 765 | 1HD2 | LEU A | 54149.455 | -7.099 | 1.811 | 1.00 | 0.00 H |
| ATOM | 766 2 | 2HD2 | LEU A | 54150.578 | -7.692 | 0.589 | 1.00 | 0.00 H |
| ATOM | 767 | 3HD2 | LEU A | 54149.962 | -6.043 | 0.492 | 1.00 | 0.00 H |
| ATOM | 768 | N | GLU A | 55149.864 | -7.752 | 6.128 | 1.00 | 0.00 N |
| ATOM | 769 | CA | GLU A | 55149.920 | -8.408 | 7.429 | 1.00 | 0.00 C |
| ATOM | 770 | C | GLU A | 55151.075 | -9.402 | 7.489 | 1.00 | 0.00 C |
| ATOM | 771 | О | GLU A | 55151.677 | -9.606 | 8.543 | 1.00 | 0.00 O |
| ATOM | 772 | СВ | GLU A | 55148.600 | -9.124 | 7.719 | 1.00 | 0.00 C |
| ATOM | 773 | CG | GLU A | 55147.559 | -8.237 | 8.381 | 1.00 | 0.00 C |
| ATOM | 774 | CD | GLU A | 55146.145 | -8.576 | 7.952 | 1.00 | 0.00 C |
| ATOM | 775 | OE1 | GLU A | 55145.281 | -7.675 | 7.989 | 1.00 | 0.00 O |
| ATOM | 776 | OE2 | GLU A | 55145.902 | -9.743 | 7.576 | 1.00 | 0.00 O |
| ATOM | 777 | Н | GLU A | 55149.191 | -8.038 | 5.477 | 1.00 | 0.00 H |
| ATOM | 778 | HA | GLU A | 55150.077 | -7.646 | 8.178 | 1.00 | 0.00 H |
| ATOM | 779 | 1HB | GLU A | 55148.191 | -9.491 | 6.789 | 1.00 | 0.00 H |
| ATOM | 780 2 | 2HB | GLU A | 55148.794 | -9.962 | 8.371 | 1.00 | 0.00 H |
| ATOM | 781 | 1HG | GLU A | 55147.631 | -8.356 | 9.452 | 1.00 | 0.00 H |
| ATOM | 782 | 2HG | GLU A | 55147.762 | -7.209 | 8.120 | 1.00 | 0.00 H |
| ATOM | 783 | N | ASPA | 56151.380 | -10.017 | 6.351 | 1.00 | 0.00 N |
| ATOM | 784 | CA | ASP A | 56152.464 | -10.989 | 6.275 | 1.00 | 0.00 C |
| ATOM | 785 | C | ASPA | 56153.720 - | 10.358 | 5.682 | 1.00 | 0.00 C |
| ATOM | 786 | О | ASPA | 56153.639 | -9.461 | 4.844 | 1.00 | 0.00 O |
| ATOM | 787 | CB | ASPA | 56152.038 | -12.194 | 5.434 | 1.00 | 0.00 C |
| ATOM | 788 | CG | ASPA | 56152.656 | -13.489 | 5.924 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASP A | 56151.930 - | 14.502 | 5.999 | 1.00 | 0.00 O |

| ATOM | 790 | OD2 | 2 ASP A | 56153.866 | -13.489 | 6.233 | 1.00 | 0.00 O |
|------|-------|-----|---------|-----------|---------|-------|------|--------|
| ATOM | 791 | Н | ASPA | 56150.865 | -9.811 | 5.544 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.682 | -11.322 | 7.278 | 1.00 | 0.00 H |
| ATOM | 793 | HB | ASPA | 56150.963 | -12.292 | 5.474 | 1.00 | 0.00 H |
| ATOM | 794 2 | 2HB | ASPA | 56152.343 | -12.036 | 4.409 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.880 | -10.835 | 6.122 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57156.153 | -10.318 | 5.635 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57156.464 | -10.862 | 4.244 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57157.189 | -11.845 | 4.098 | 1.00 | 0.00 O |
| ATOM | 799 | CB | GLU A | 57157.281 | -10.684 | 6.601 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.059 | -10.172 | 8.016 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57156.643 | -11.271 | 8.975 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57155.525 | -11.806 | 8.817 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57157.435 | -11.596 | 9.885 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.880 | -11.552 | 6.790 | 1.00 | 0.00 H |
| ATOM | 805 | HA | GLU A | 57156.074 | -9.242 | 5.579 | 1.00 | 0.00 H |
| ATOM | 806 1 | HB | GLU A | 57157.370 | -11.760 | 6.641 | 1.00 | 0.00 H |
| ATOM | 807 2 | HB | GLU A | 57158.206 | -10.268 | 6.231 | 1.00 | 0.00 H |
| ATOM | 808 1 | HG | GLU A | 57157.977 | -9.732 | 8.374 | 1.00 | 0.00 H |
| ATOM | 809 2 | HG | GLU A | 57156.284 | -9.419 | 7.995 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58155.911 | -10.214 | 3.224 | 1.00 | 0.00 N |
| ATOM | 811 | CA | CYS A | 58156.129 | -10.631 | 1.844 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58157.505 | -10.192 | 1.354 | 1.00 | 0.00 C |
| ATOM | 813 | O | CYS A | 58157.859 | -9.016 | 1.437 | 1.00 | 0.00 O |
| ATOM | 814 | CB | CYS A | 58155.043 | -10.051 | 0.935 | 1.00 | 0.00 C |
| ATOM | 815 | SG | CYS A | 58153.516 | -11.020 | 0.901 | 1.00 | 0.00 S |
| ATOM | 816 | Н | CYS A | 58155.341 | -9.436 | 3.404 | 1.00 | 0.00 H |

| ATOM | 817 | HA | CYSA | 58156.076 | -11.709 | 1.812 | 1.00 | 0.00 H |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 818 | 1HB | CYS A | 58154.793 | -9.057 | 1.275 | 1.00 | 0.00 H |
| ATOM | 819 2 | 2HB | CYS A | 58155.420 | -9.996 | -0.075 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYS A | 58153.511 | -11.593 | 1.672 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALAA | 59158.278 | -11.145 | 0.842 | 1.00 | 0.00 N |
| ATOM | 822 | CA | ALA A | 59159.615 | -10.857 | 0.338 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59159.552 | -10.057 | -0.958 | 1.00 | 0.00 C |
| ATOM | 824 | O | ALAA | 59159.080 | -10.551 | -1.981 | 1.00 | 0.00 O |
| ATOM | 825 | СВ | ALAA | 59160.388 | -12.149 | 0.126 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALA A | 59157.939 | -12.064 | 0.802 | 1.00 | 0.00 H |
| ATOM | 827 | НА | ALA A | 59160.133 | -10.274 | 1.085 | 1.00 | 0.00 H |
| ATOM | 828 | IНВ | ALA A | 59159.764 - | 12.860 | -0.395 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59160.677 - | 12.557 | 1.084 | 1.00 | 0.00 H |
| ATOM | 830 3 | ЗНВ | ALA A | 59161.272 - | 11.948 | -0.460 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60160.031 | -8.818 | -0.907 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60160.020 | -7.970 | -2.084 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60159.553 | -6.560 | -1.778 | 1.00 | 0.00 C |
| ATOM | 834 | O | GLY A | 60159.945 | -5.608 | -2.455 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60160.396 | -8.478 | -0.063 | 1.00 | 0.00 H |
| ATOM | 836 | lНА | GLY A | 60161.020 | -7.926 | -2.491 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60159.362 | -8.403 | -2.821 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYS A | 61158.713 | -6.425 | -0.757 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.192 | -5.122 | -0.363 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.189 | -4.380 | 0.519 | 1.00 | 0.00 C |
| ATOM | 841 | O | CYS A | 61160.222 | -4.931 | 0.904 | 1.00 | 0.00 O |
| ATOM | 842 | CB | CYS A | 61156.861 | -5.283 | 0.375 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYS A | 61155.608 | -6.197 | -0.553 | 1.00 | 0.00 S |

| ATOM | 844 | Н | CYS A | 61158.438 | -7.221 | -0.257 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|---------|--------|------|--------|
| ATOM | 845 | НА | CYS A | 61158.026 | -4.545 | -1.262 | 1.00 | 0.00 H |
| ATOM | 846 | 1HB | CYS A | 61157.035 | -5.812 | 1.301 | 1.00 | 0.00 H |
| ATOM | 847 | 2HB | CYS A | 61156.460 | -4.305 | 0.595 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61154.811 | -5.662 | -0.582 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.876 | -3.128 | 0.835 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.746 | -2.310 | 1.673 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.171 | -2.169 | 3.078 | 1.00 | 0.00 C |
| ATOM | 852 | Ο | THR A | 62158.132 | -2.748 | 3.397 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62159.940 | -0.929 | 1.047 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.694 | -0.283 | 0.860 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62160.641 | -0.973 | -0.294 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62158.040 | -2.744 | 0.498 | 1.00 | 0.00 H |
| ATOM | 857 | HA | THR A | 62160.704 | -2.805 | 1.737 | 1.00 | 0.00 H |
| ATOM | 858 | HB | THR A | 62160.540 | -0.325 | 1.712 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62158.840 | 0.602 | 0.518 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62160.440 | -1.919 | -0.774 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62161.705 | -0.862 | -0.148 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62160.277 | -0.169 | -0.917 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63159.853 | -1.394 | 3.916 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASP A | 63159.410 | -1.175 | 5.289 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.661 | 0.148 | 5.414 | 1.00 | 0.00 C |
| ATOM | 866 | O | ASPA | 63158.703 | 0.800 | 6.457 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASP A | 63160.606 | -1.189 | 6.241 | 1.00 | 0.00 C |
| ATOM | 868 | CG | ASPA | 63161.704 | -0.240 | 5.805 | 1.00 | 0.00 C |
| ATOM | 869 | OD1 | ASPA | 63161.752 | 0.893 | 6.328 | 1.00 | 0.00 O |
| ATOM | 870 | OD2 | ASPA | 63162.517 | - 0.629 | 4.939 | 1.00 | 0.00 O |

| ATOM | 871 | Н | ASPA | 63160.674 | -0.958 | 3.604 | 1.00 | 0.00 H |
|------|-----|--------|-------|-----------|--------|--------|------|--------|
| ATOM | 872 | HA | ASPA | 63158.741 | -1.980 | 5.553 | 1.00 | 0.00 H |
| ATOM | 873 | 1HB | ASPA | 63160.276 | -0.899 | 7.227 | 1.00 | 0.00 H |
| ATOM | 874 | 2HB | ASPA | 63161.013 | -2.189 | 6.282 | 1.00 | 0.00 H |
| ATOM | 875 | N | GLY A | 64157.976 | 0.538 | 4.344 | 1.00 | 0.00 N |
| ATOM | 876 | CA | GLY A | 64157.227 | 1.781 | 4.356 | 1.00 | 0.00 C |
| ATOM | 877 | C | GLY A | 64157.980 | 2.918 | 3.692 | 1.00 | 0.00 C |
| ATOM | 878 | O | GLY A | 64158.006 | 4.037 | 4.204 | 1.00 | 0.00 O |
| ATOM | 879 | Н | GLY A | 64157.978 | -0.022 | 3.540 | 1.00 | 0.00 H |
| ATOM | 880 | 1HA | GLY A | 64156.292 | 1.631 | 3.836 | 1.00 | 0.00 H |
| ATOM | 881 | 2HA | GLY A | 64157.018 | 2.053 | 5.380 | 1.00 | 0.00 H |
| ATOM | 882 | N | THR A | 65158.594 | 2.630 | 2.549 | 1.00 | 0.00 N |
| ATOM | 883 | CA | THR A | 65159.351 | 3.636 | 1.814 | 1.00 | 0.00 C |
| ATOM | 884 | C | THR A | 65159.077 | 3.536 | 0.317 | 1.00 | 0.00 C |
| ATOM | 885 | O | THR A | 65159.346 | 2.511 | -0.307 | 1.00 | 0.00 O |
| ATOM | 886 | CB | THR A | 65160.848 | 3.475 | 2.081 | 1.00 | 0.00 C |
| ATOM | 887 | OG1 | THR A | 65161.266 | 2.148 | 1.810 | 1.00 | 0.00 O |
| ATOM | 888 | CG2 | THR A | 65161.239 | 3.795 | 3.508 | 1.00 | 0.00 C |
| ATOM | 889 | Н | THR A | 65158.536 | 1.720 | 2.192 | 1.00 | 0.00 H |
| ATOM | 890 | НА | THR A | 65159.035 | 4.608 | 2.162 | 1.00 | 0.00 H |
| ATOM | 891 | HB | THR A | 65161.394 | 4.143 | 1.431 | 1.00 | 0.00 H |
| ATOM | 892 | HG1 | THR A | 65161.056 | 1.927 | 0.900 | 1.00 | 0.00 H |
| ATOM | 893 | 1HG2 | THR A | 65160.578 | 4.555 | 3.900 | 1.00 | 0.00 H |
| ATOM | 894 | 2HG2 ' | THR A | 65162.256 | 4.158 | 3.530 | 1.00 | 0.00 H |
| ATOM | 895 | 3HG2 | THR A | 65161.162 | 2.904 | 4.112 | 1.00 | 0.00 H |
| ATOM | 896 | N | PHE A | 66158.540 | 4.610 | -0.254 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.230 | 4.645 | -1.678 | 1.00 | 0.00 C |

| ATOM | 898 | C | PHE A | 66159.285 | 5.435 | -2.446 | 1.00 | 0.00 C |
|-------|-------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 899 | Ο | PHE A | 66159.348 | 6.660 | -2.351 | 1.00 | 0.00 O |
| ATOM | 900 | СВ | PHE A | 66156.848 | 5.261 | -1.905 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.258 | 4.935 | -3.248 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.882 | 5.945 | -4.118 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66156.081 | 3.618 | -3.638 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.340 | 5.647 | -5.354 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.538 | 3.314 | -4.873 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66155.167 | 4.330 | -5.732 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.348 | 5.398 | 0.296 | 1.00 | 0.00 H |
| ATOM | 908 | HA | PHE A | 66158.224 | 3.628 | -2.040 | 1.00 | 0.00 H |
| ATOM | 909 | lНВ | PHE A | 66156.171 | 4.898 | -1.148 | 1.00 | 0.00 H |
| ATOM | 910 2 | 2HB | PHE A | 66156.925 | 6.337 | -1.827 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66156.018 | 6.976 | -3.824 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.370 | 2.822 | -2.968 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66155.051 | 6.445 | -6.023 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.404 | 2.283 | -5.166 | 1.00 | 0.00 H |
| ATOM | 915 | HZ | PHE A | 66154.743 | 4.096 | -6.696 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67160.111 | 4.724 | -3.207 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67161.164 | 5.358 | -3.991 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67162.128 | 6.124 | -3.090 | 1.00 | 0.00 C |
| ATOM | 919 | O | ARG A | 67162.576 | 7.219 | -3.430 | 1.00 | 0.00 O |
| ATOM. | 920 | CB | ARG A | 67160.557 | 6.304 | -5.029 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67159.739 | 5.593 | -6.096 | 1.00 | 0.00 C |
| ATOM | 922 | CD | ARG A | 67160.131 | 6.041 | -7.495 | 1.00 | 0.00 C |
| ATOM | 923 | NE | ARG A | 67161.016 | 5.080 | -8.150 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67161.773 | 5.370 | -9.206 | 1.00 | 0.00 C |

| ATOM | 925 | NH1 | ARG A | 67161.755 | 6.590 | -9.731 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 926 | NH2 | ARG A | 67162.549 | 4.437 | -9.741 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67160.011 | 3.750 | -3.241 | 1.00 | 0.00 H |
| ATOM | 928 | HA | ARG A | 67161.711 | 4.580 | -4.503 | 1.00 | 0.00 H |
| ATOM | 929 | 1HB | ARG A | 67159.912 | 7.008 | -4.523 | 1.00 | 0.00 H |
| ATOM | 930 | 2HB | ARG A | 67161.353 | 6.846 | -5.516 | 1.00 | 0.00 H |
| ATOM | 931 | 1HG | ARG A | 67159.904 | 4.529 | -6.012 | 1.00 | 0.00 H |
| ATOM | 932 | 2HG | ARG A | 67158.693 | 5.810 | -5.938 | 1.00 | 0.00 H |
| ATOM | 933 | 1HD | ARG A | 67159.236 | 6.154 | -8.088 | 1.00 | 0.00 H |
| ATOM | 934 | 2HD | ARG A | 67160.638 | 6.994 | -7.425 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67161.048 | 4.172 | -7.783 | 1.00 | 0.00 H |
| ATOM | 936 | 1HH1 | ARG A | 67161.172 | 7.297 | -9.333 | 1.00 | 0.00 H |
| ATOM | 937 | 2HH1 | ARG A | 67162.325 | 6.801 - | 10.524 | 1.00 | 0.00 H |
| ATOM | 938 | 1HH2 | ARG A | 67162.566 | 3.516 | -9.351 | 1.00 | 0.00 H |
| ATOM | 939 | 2HH2 | ARG A | 67163.117 | 4.653 - | 10.535 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.443 | 5.540 | -1.939 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.351 | 6.182 | -1.006 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.706 | 7.342 | -0.275 | 1.00 | 0.00 C |
| ATOM | 943 | O | GLY A | 68163.385 | 8.287 | 0.127 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68162.055 | 4.667 | -1.721 | 1.00 | 0.00 H |
| ATOM | 945 | 1HA | GLY A | 68163.679 | 5.452 | -0.281 | 1.00 | 0.00 H |
| ATOM | 946 2 | 2HA | GLY A | 68164.210 | 6.546 | -1.550 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.389 | 7.272 | -0.102 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.651 | 8.325 | 0.585 | 1.00 | 0.00 C |
| ATOM | 949 | C | THR A | 69159.735 | 7.739 | 1.654 | 1.00 | 0.00 C |
| ATOM | 950 | O | THR A | 69158.604 | 7.347 | 1.369 | 1.00 | 0.00 O |
| ATOM | 951 | CB | THR A | 69159.829 | 9.137 | -0.417 | 1.00 | 0.00 C |

| ATOM | 952 | OG1 | THR A | 69160.590 | 9.421 | -1.578 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 953 | CG2 | THR A | 69159.336 | 10.454 | 0.141 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.902 | 6.493 | -0.445 | 1.00 | 0.00 H |
| ATOM | 955 | НА | THR A | 69161.368 | 8.976 | 1.061 | 1.00 | 0.00 H |
| ATOM | 956 | НВ | THR A | 69158.965 | 8.558 | -0.711 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.292 | 10.038 | -1.358 | 1.00 | 0.00 H |
| ATOM | 958 | 1HG2 | THR A | 69159.985 | 11.252 | -0.190 | 1.00 | 0.00 H |
| ATOM | 959 | 2HG2 | THR A | 69159.340 | 10.412 | 1.220 | 1.00 | 0.00 H |
| ATOM | 960 | 3HG2 | THR A | 69158.331 | 10.639 | -0.208 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.232 | 7.682 | 2.886 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.457 | 7.143 | 3.998 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.310 | 8.077 | 4.365 | 1.00 | 0.00 C |
| ATOM | 964 | Ο | ARG A | 70158.529 | 9.234 | 4.725 | 1.00 | 0.00 O |
| ATOM | 965 | CB | ARG A | 70160.359 | 6.919 | 5.213 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70159.662 | 6.210 | 6.364 | 1.00 | 0.00 C |
| ATOM | 967 | CD | ARG A | 70159.925 | 6.903 | 7.691 | 1.00 | 0.00 C |
| ATOM | 968 | NE | ARG A | 70159.851 | 5.977 | 8.819 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70160.254 | 6.275 | 10.051 | 1.00 | 0.00 C |
| ATOM | 970 | NH1 | ARG A | 70160.761 | 7.472 | 10.320 | 1.00 | 0.00 N |
| ATOM | 971 | NH2 | ARG A | 70160.151 | 5.374 | 11.018 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.141 | 8.009 | 3.050 | 1.00 | 0.00 H |
| ATOM | 973 | HA | ARG A | 70159.048 | 6.193 | 3.686 | 1.00 | 0.00 H |
| ATOM | 974 | 1HB | ARG A | 70161.208 | 6.324 | 4.913 | 1.00 | 0.00 H |
| ATOM | 975 | 2HB | ARGA | 70160.709 | 7.878 | 5.567 | 1.00 | 0.00 H |
| ATOM | 976 | 1HG | ARG A | 70158.599 | 6.203 | 6.178 | 1.00 | 0.00 H |
| ATOM | 977 | 2HG | ARG A | 70160.026 | 5.194 | 6.421 | 1.00 | 0.00 H |
| ATOM | 978 | 1HD | ARG A | 70160.912 | 7.343 | 7.663 | 1.00 | 0.00 H |

| ATOM | 979 | 2HD | ARG A | 70159.189 | 7.682 | 7.827 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 980 | HE | ARG A | 70159.482 | 5.085 | 8.647 | 1.00 | 0.00 H |
| ATOM | 981 | 1HH1 | ARG A | 70160.841 | 8.157 | 9.595 | 1.00 | 0.00 H |
| ATOM | 982 | 2HH1 | ARG A | 70161.062 | 7.690 | 11.248 | 1.00 | 0.00 H |
| ATOM | 983 | 1HH2 | ARG A | 70159.771 | 4.470 | 10.820 | 1.00 | 0.00 H |
| ATOM | 984 | 2HH2 | ARG A | 70160.454 | 5.598 | 11.945 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.086 | 7.567 | 4.275 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71155.903 | 8.356 | 4.599 | 1.00 | 0.00 C |
| ATOM | 987 | C | TYR A | 71155.381 | 8.004 | 5.988 | 1.00 | 0.00 C |
| ATOM | 988 | Ο | TYR A | 71154.877 | 8.865 | 6.710 | 1.00 | 0.00 O |
| ATOM | 989 | CB | TYR A | 71154.808 | 8.125 | 3.556 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.153 | 8.667 | 2.187 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.218 | 7.826 | 1.083 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.413 | 10.018 | 1.998 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.533 | 8.316 | -0.170 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.727 | 10.517 | 0.748 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.786 | 9.662 | -0.332 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71156.099 | 10.155 | -1.578 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71156.976 | 6.638 | 3.983 | 1.00 | 0.00 H |
| ATOM | 998 | HA | TYR A | 71156.187 | 9.397 | 4.587 | 1.00 | 0.00 H |
| ATOM | 999 | 1HB | TYR A | 71154.633 | 7.064 | 3.458 | 1.00 | 0.00 H |
| ATOM | 1000 | 2HB | TYR A | 71153.901 | 8.607 | 3.886 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.019 | 6.773 | 1.213 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYR A | 71155.367 | 10.685 | 2.846 | 1.00 | 0.00 H |
| ATOM | 1003 | HE1 | TYR A | 71155.578 | 7.646 | -1.016 | 1.00 | 0.00 H |
| ATOM | 1004 | HE2 | TYR A | 71155.926 | 11.571 | 0.622 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71155.373 | 9.983 | -2.182 | 1.00 | 0.00 H |

| ATOM | 1006 | N | PHE A | 72155.504 | 6.733 | 6.357 | 1.00 | 0.00 N |
|------|--------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 1007 | CA | PHE A | 72155.045 | 6.266 | 7.659 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.020 | 5.251 | 8.248 | 1.00 | 0.00 C |
| ATOM | 1009 | О | PHE A | 72157.052 | 4.949 | 7.649 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72153.653 | 5.642 | 7.538 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72153.543 | 4.631 | 6.433 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72153.294 | 5.033 | 5.130 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72153.689 | 3.278 | 6.696 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72153.193 | 4.104 | 4.111 | 1.00 | 0.00 C |
| ATOM | 1015 | CE2 | PHE A | 72153.588 | 2.345 | 5.682 | 1.00 | 0.00 C |
| ATOM | 1016 | CZ | PHE A | 72153.340 | 2.759 | 4.388 | 1.00 | 0.00 C |
| ATOM | 1017 | Н | PHE A | 72155.914 | 6.094 | 5.737 | 1.00 | 0.00 H |
| ATOM | 1018 | НА | PHE A | 72154.990 | 7.120 | 8.317 | 1.00 | 0.00 H |
| ATOM | 1019 | 1HB | PHE A | 72153.406 | 5.147 | 8.465 | 1.00 | 0.00 H |
| ATOM | 1020 2 | 2HB | PHE A | 72152.931 | 6.422 | 7.349 | 1.00 | 0.00 H |
| ATOM | 1021 | HD1 | PHE A | 72153.179 | 6.084 | 4.913 | 1.00 | 0.00 H |
| ATOM | 1022 | HD2 | PHE A | 72153.884 | 2.954 | 7.708 | 1.00 | 0.00 H |
| ATOM | 1023 | HE1 | PHE A | 72152.997 | 4.431 | 3.101 | 1.00 | 0.00 H |
| ATOM | 1024 | HE2 | PHE A | 72153.705 | 1.294 | 5.901 | 1.00 | 0.00 H |
| ATOM | 1025 | HZ | PHE A | 72153.262 | 2.032 | 3.593 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73155.687 | 4.731 | 9.424 | 1.00 | 0.00 N |
| ATOM | 1027 | CA | THR A | 73156.534 | 3.750 | 10.094 | 1.00 | 0.00 C |
| ATOM | 1028 | C | THR A | 73155.833 | 2.399 | 10.188 | 1.00 | 0.00 C |
| ATOM | 1029 | О | THR A | 73154.813 | 2.263 | 10.862 | 1.00 | 0.00 O |
| ATOM | 1030 | СВ | THR A | 73156.909 | 4.241 | 11.493 | 1.00 | 0.00 C |
| ATOM | 1031 | OG1 | THR A | 73157.700 | 3.278 | 12.167 | 1.00 | 0.00 O |
| ATOM | 1032 | CG2 | THR A | 73155.709 | 4.539 | 12.365 | 1.00 | 0.00 C |

| ATOM | 1033 | Н | THR A | 73154.851 | 5.012 | 9.852 | 1.00 | 0.00 H |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1034 | НА | THR A | 73157.434 | 3.636 | 9.510 | 1.00 | 0.00 H |
| ATOM | 1035 | HB | THR A | 73157.486 | 5.150 | 11.401 | 1.00 | 0.00 H |
| ATOM | 1036 | HG1 | THR A | 73158.049 | 3.660 | 12.976 | 1.00 | 0.00 H |
| ATOM | 1037 | HG2 | THR A | 73155.202 | 3.617 | 12.608 | 1.00 | 0.00 H |
| ATOM | 1038 2 | 2HG2 | THR A | 73155.032 | 5.192 | 11.834 | 1.00 | 0.00 H |
| ATOM | 1039 | 3HG2 | THR A | 73156.035 | 5.021 | 13.274 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYSA | 74156.388 | 1.402 | 9.505 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74155.816 | 0.060 | 9.512 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74156.913 | -0.999 | 9.554 | 1.00 | 0.00 C |
| ATOM | 1043 | O | CYS A | 74158.096 | -0.687 | 9.422 | 1.00 | 0.00 O |
| ATOM | 1044 | CB | CYS A | 74154.939 | -0.148 | 8.276 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYSA | 74153.237 | 0.427 | 8.475 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYS A | 74157.201 | 1.572 | 8.985 | 1.00 | 0.00 H |
| ATOM | 1047 | НА | CYSA | 74155.205 | -0.035 | 10.396 | 1.00 | 0.00 H |
| ATOM | 1048 | HВ | CYS A | 74155.370 | 0.387 | 7.443 | 1.00 | 0.00 H |
| ATOM | 1049 2 | 2HB | CYS A | 74154.905 | -1.202 | 8.042 | 1.00 | 0.00 H |
| ATOM | 1050 | ĤG | CYS A | 74152.753 | 0.204 | 7.676 | 1.00 | 0.00 H |
| ATOM | 1051 | N | ALA A | 75156.512 | -2.252 | 9.739 | 1.00 | 0.00 N |
| ATOM | 1052 | CA | ALA A | 75157.461 | -3.357 | 9.799 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75158.197 | -3.521 | 8.474 | 1.00 | 0.00 C |
| ATOM | 1054 | O | ALA A | 75157.960 | -2.774 | 7.524 | 1.00 | 0.00 O |
| ATOM | 1055 | CB | ALAA | 75156.745 | -4.647 | 10.170 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALA A | 75155.554 | -2.438 | 9.837 | 1.00 | 0.00 H |
| ATOM | 1057 | НА | ALA A | 75158.180 | -3.137 | 10.574 | 1.00 | 0.00 H |
| ATOM | 1058 | lНВ | ALA A | 75156.801 | -4.796 | 11.238 | 1.00 | 0.00 H |
| ATOM | 1059 | 2НВ | ALA A | 75157.215 | -5.478 | 9.665 | 1.00 | 0.00 H |

| ATOM | 1060 | 3HB | ALA A | 75155.709 | -4.583 | 9.869 | 1.00 | 0.00 H | |
|------|------|------|-------|-----------|--------|-------|------|--------|--|
| ATOM | 1061 | N | LEU A | 76159.091 | -4.502 | 8.416 | 1.00 | 0.00 N | |
| ATOM | 1062 | CA | LEU A | 76159.862 | -4.764 | 7.206 | 1.00 | 0.00 C | |
| ATOM | 1063 | C | LEU A | 76159.161 | -5.793 | 6.326 | 1.00 | 0.00 C | |
| ATOM | 1064 | О | LEU A | 76158.560 | -6.745 | 6.825 | 1.00 | 0.00 O | |
| ATOM | 1065 | CB | LEU A | 76161.265 | -5.256 | 7.566 | 1.00 | 0.00 C | |
| ATOM | 1066 | CG | LEU A | 76162.272 | -4.153 | 7.899 | 1.00 | 0.00 C | |
| ATOM | 1067 | CD1 | LEU A | 76163.265 | -4.636 | 8.945 | 1.00 | 0.00 C | |
| ATOM | 1068 | CD2 | LEU A | 76162.999 | -3.700 | 6.642 | 1.00 | 0.00 C | |
| ATOM | 1069 | Н | LEU A | 76159.236 | -5.064 | 9.206 | 1.00 | 0.00 H | |
| ATOM | 1070 | HA | LEU A | 76159.945 | -3.836 | 6.659 | 1.00 | 0.00 H | |
| ATOM | 1071 | 1HB | LEU A | 76161.185 | -5.912 | 8.421 | 1.00 | 0.00 H | |
| ATOM | 1072 | 2HB | LEU A | 76161.650 | -5.823 | 6.733 | 1.00 | 0.00 H | |
| ATOM | 1073 | HG | LEU A | 76161.745 | -3.304 | 8.307 | 1.00 | 0.00 H | |
| ATOM | 1074 | 1HD1 | LEU A | 76164.124 | -5.069 | 8.454 | 1.00 | 0.00 H | |
| ATOM | 1075 | 2HD1 | LEU A | 76162.795 | -5.380 | 9.572 | 1.00 | 0.00 H | |
| ATOM | 1076 | 3HD1 | LEU A | 76163.582 | -3.801 | 9.554 | 1.00 | 0.00 H | |
| ATOM | 1077 | 1HD2 | LEU A | 76162.395 | -3.926 | 5.775 | 1.00 | 0.00 H | |
| ATOM | 1078 | 2HD2 | LEU A | 76163.945 | -4.216 | 6.567 | 1.00 | 0.00 H | |
| ATOM | 1079 | 3HD2 | LEU A | 76163.173 | -2.636 | 6.690 | 1.00 | 0.00 H | |
| ATOM | 1080 | N | LYS A | 77159.241 | -5.595 | 5.014 | 1.00 | 0.00 N | |
| ATOM | 1081 | CA | LYS A | 77158.615 | -6.506 | 4.063 | 1.00 | 0.00 C | |
| ATOM | 1082 | C | LYS A | 77157.102 | -6.545 | 4.261 | 1.00 | 0.00 C | |
| ATOM | 1083 | O | LYS A | 77156.473 | -7.591 | 4.107 | 1.00 | 0.00 O | |
| ATOM | 1084 | СВ | LYS A | 77159.196 | -7.914 | 4.213 | 1.00 | 0.00 C | |
| ATOM | 1085 | CG | LYS A | 77160.695 | -7.980 | 3.971 | 1.00 | 0.00 C | |
| ATOM | 1086 | CD | LYS A | 77161.038 | -7.712 | 2.515 | 1.00 | 0.00 C | |

| ATOM | 1087 | CE | LYS A | 77162.514 | -7.398 | 2.339 | 1.00 | 0.00 C |
|-------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1088 | NZ | LYS A | 77163.360 | -8.619 | 2.449 | 1.00 | 0.00 N |
| ATOM | 1089 | Н | LYS A | 77159.734 | -4.817 | 4.677 | 1.00 | 0.00 H |
| ATOM | 1090 | НА | LYS A | 77158.826 | -6.143 | 3.069 | 1.00 | 0.00 H |
| ATOM | 1091 | lНВ | LYS A | 77158.998 | -8.268 | 5.213 | 1.00 | 0.00 H |
| ATOM | 1092 | 2HB | LYS A | 77158.709 | -8.569 | 3.505 | 1.00 | 0.00 H |
| ATOM | 1093 | HG | LYS A | 77161.183 | -7.239 | 4.587 | 1.00 | 0.00 H |
| ATOM | 1094 2 | 2HG | LYS A | 77161.050 | -8.965 | 4.240 | 1.00 | 0.00 H |
| ATOM | 1095 | IHD | LYS A | 77160.794 | -8.586 | 1.931 | 1.00 | 0.00 H |
| ATOM | 1096 2 | 2HD | LYS A | 77160.456 | -6.871 | 2.167 | 1.00 | 0.00 H |
| ATOM | 1097 | HE | LYS A | 77162.662 | -6.956 | 1.364 | 1.00 | 0.00 H |
| ATOM | 1098 2 | 2HE | LYS A | 77162.813 | -6.693 | 3.101 | 1.00 | 0.00 H |
| ATOM | 1099 | ΙHΖ | LYS A | 77162.813 | -9.459 | 2.167 | 1.00 | 0.00 H |
| ATOM | 1100 2 | 2HZ | LYS A | 77163.682 | -8.743 | 3.430 | 1.00 | 0.00 H |
| ATOM | 1101 3 | BHZ | LYS A | 77164.191 | -8.536 | 1.831 | 1.00 | 0.00 H |
| ATOM | 1102 | N | LYS A | 78156.526 | -5.398 | 4.602 | 1.00 | 0.00 N |
| ATOM | 1103 | CA | LYS A | 78155.087 | -5.300 | 4.821 | 1.00 | 0.00 C |
| ATOM, | 1104 | C | LYS A | 78154.565 | -3.928 | 4.407 | 1.00 | 0.00 C |
| ATOM | 1105 | O | LYS A | 78153.672 | -3.373 | 5.047 | 1.00 | 0.00 O |
| ATOM | 1106 | СВ | LYS A | 78154.754 | -5.564 | 6.291 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.276 | -6.897 | 6.803 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78155.037 | -7.051 | 8.296 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYS A | 78153.738 | -7.786 | 8.580 | 1.00 | 0.00 C |
| ATOM | 1110 | NZ | LYS A | 78153.489 | -7.930 | 10.040 | 1.00 | 0.00 N |
| ATOM | 1111 | Н | LYS A | 78157.081 | -4.597 | 4.709 | 1.00 | 0.00 H |
| ATOM | 1112 | HA | LYS A | 78154.609 | -6.053 | 4.212 | 1.00 | 0.00 H |
| ATOM | 1113 | НВ | LYS A | 78155.187 | -4.778 | 6.892 | 1.00 | 0.00 H |

| ATOM | 11142 | 2HB | LYS A | 78153.682 | -5.551 | 6.413 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 1115 | IHG | LYS A | 78154.768 | -7.695 | 6.283 | 1.00 | 0.00 H |
| ATOM | 11162 | 2HG | LYS A | 78156.337 | -6.956 | 6.609 | 1.00 | 0.00 H |
| ATOM | 1117 | IHD | LYS A | 78155.857 | -7.608 | 8.726 | 1.00 | 0.00 H |
| ATOM | 11182 | 2HD | LYS A | 78154.992 | -6.070 | 8.746 | 1.00 | 0.00 H |
| ATOM | 1119 | HE | LYS A | 78152.923 | -7.233 | 8.138 | 1.00 | 0.00 H |
| ATOM | 1120 2 | 2HE | LYS A | 78153.790 | -8.768 | 8.132 | 1.00 | 0.00 H |
| ATOM | 1121 | ΙHZ | LYS A | 78152.472 | -7.847 | 10.240 | 1.00 | 0.00 H |
| ATOM | 1122 2 | 2HZ | LYSA | 78153.995 | -7.189 | 10.566 | 1.00 | 0.00 H |
| ATOM | 1123 3 | BHZ | LYS A | 78153.820 | -8.860 | 10.369 | 1.00 | 0.00 H |
| ATOM | 1124 | N | ALA A | 79155.130 | -3.385 | 3.333 | 1.00 | 0.00 N |
| ATOM | 1125 | CA | ALA A | 79154.722 | -2.078 | 2.834 | 1.00 | 0.00 C |
| ATOM | 1126 | C | ALA A | 79154.661 | - 2.066 | 1.311 | 1.00 | 0.00 C |
| ATOM | 1127 | O | ALA A | 79155.692 | -2.045 | 0.638 | 1.00 | 0.00 O |
| ATOM | 1128 | CB | ALA A | 79155.673 | -1.002 | 3.334 | 1.00 | 0.00 C |
| ATOM | 1129 | Н | ALA A | 79155.838 | -3.876 | 2.865 | 1.00 | 0.00 H |
| ATOM | 1130 | НА | ALA A | 79153.737 | -1.864 | 3.225 | 1.00 | 0.00 H |
| ATOM | 1131 1 | НВ | ALA A | 79156.179 | -1.352 | 4.222 | 1.00 | 0.00 H |
| ATOM | 1132 2 | 2HB | ALA A | 79155.115 | -0.107 | 3.567 | 1.00 | 0.00 H |
| ATOM | 1133 3 | НВ | ALA A | 79156.402 | -0.782 | 2.568 | 1.00 | 0.00 H |
| ATOM | 1134 | N | LEU A | 80153.445 | -2.077 | 0.772 | 1.00 | 0.00 N |
| ATOM | 1135 | CA | LEU A | 80153.250 | -2.068 | -0.674 | 1.00 | 0.00 C |
| ATOM | 1136 | C | LEU A | 80152.372 | -0.893 | -1.095 | 1.00 | 0.00 C |
| ATOM | 1137 | О | LEU A | 80151.191 | -0.835 | -0.752 | 1.00 | 0.00 O |
| ATOM | 1138 | СВ | LEU A | 80152.617 | -3.383 | -1.131 | 1.00 | 0.00 C |
| ATOM | 1139 | CG | LEU A | 80152.301 | -3.464 | -2.626 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.582 | -3.431 | -3.445 | 1.00 | 0.00 C |

| | ATOM | 1141 | CD2 | LEU A | 80151.501 | -4.721 | -2.933 | 1.00 | 0.00 C |
|-----|------|--------|------|-------|-----------|--------|--------|------|--------|
| | ATOM | 1142 | Н | LEU A | 80152.662 | -2.093 | 1.360 | 1.00 | 0.00 H |
| . • | ATOM | 1143 | НА | LEU A | 80154.218 | -1.962 | -1.139 | 1.00 | 0.00 H |
| | ATOM | 1144 | 1HB | LEU A | 80153.294 | -4.189 | -0.883 | 1.00 | 0.00 H |
| | ATOM | 1145 | 2HB | LEU A | 80151.698 | -3.526 | -0.585 | 1.00 | 0.00 H |
| | ATOM | 1146 | HG | LEU A | 80151.704 | -2.608 | -2.907 | 1.00 | 0.00 H |
| | ATOM | 1147 | 1HD1 | LEU A | 80153.460 | -4.038 | -4.330 | 1.00 | 0.00 H |
| | ATOM | 1148 2 | 2HD1 | LEU A | 80154.399 | -3.819 | -2.852 | 1.00 | 0.00 H |
| | ATOM | 1149 | 3HD1 | LEU A | 80153.799 | -2.413 | -3.734 | 1.00 | 0.00 H |
| | ATOM | 1150 | 1HD2 | LEU A | 80151.751 | -5.074 | -3.924 | 1.00 | 0.00 H |
| | ATOM | 11512 | 2HD2 | LEU A | 80150.446 | -4.496 | -2.887 | 1.00 | 0.00 H |
| | ATOM | 1152 | 3HD2 | LEU A | 80151.739 | -5.485 | -2.209 | 1.00 | 0.00 H |
| | ATOM | 1153 | N | PHE A | 81152.956 | 0.039 | -1.839 | 1.00 | 0.00 N |
| | ATOM | 1154 | CA | PHE A | 81152.227 | 1.212 | -2.307 | 1.00 | 0.00 C |
| | ATOM | 1155 | C | PHE A | 81151.468 | 0.904 | -3.594 | 1.00 | 0.00 C |
| | ATOM | 1156 | О | PHE A | 81151.964 | 0.183 | -4.460 | 1.00 | 0.00 O |
| | ATOM | 1157 | CB | PHE A | 81153.188 | 2.379 | -2.536 | 1.00 | 0.00 C |
| | ATOM | 1158 | CG | PHE A | 81153.792 | 2.916 | -1.270 | 1.00 | 0.00 C |
| | ATOM | 1159 | CD1 | PHE A | 81154.989 | 2.410 | -0.788 | 1.00 | 0.00 C |
| | ATOM | 1160 | CD2 | PHE A | 81153.164 | 3.928 | -0.561 | 1.00 | 0.00 C |
| | ATOM | 1161 | CE1 | PHE A | 81155.547 | 2.902 | 0.377 | 1.00 | 0.00 C |
| | ATOM | 1162 | CE2 | PHE A | 81153.717 | 4.425 | 0.603 | 1.00 | 0.00 C |
| | ATOM | 1163 | CZ | PHE A | 81154.910 | 3.911 | 1.073 | 1.00 | 0.00 C |
| | ATOM | 1164 | Н | PHE A | 81153.900 | -0.064 | -2.079 | 1.00 | 0.00 H |
| ٠ | ATOM | 1165 | НА | PHE A | 81151.516 | 1.487 | -1.543 | 1.00 | 0.00 H |
| | ATOM | 1166 | 1HB | PHE A | 81153.995 | 2.052 | -3.175 | 1.00 | 0.00 H |
| | ATOM | 1167 | 2HB | PHE A | 81152.657 | 3.185 | -3.020 | 1.00 | 0.00 H |

| ATOM | 1168 | HDI | PHE A | 81155.488 | 1.622 | -1.332 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1169 | HD2 | PHE A | 81152.231 | 4.330 | -0.928 | 1.00 | 0.00 H |
| ATOM | 1170 | HE1 | PHE A | 81156.480 | 2.499 | 0.742 | 1.00 | 0.00 H |
| ATOM | 1171 | HE2 | PHE A | 81153.216 | 5.213 | 1.146 | 1.00 | 0.00 H |
| ATOM | 1172 | HZ | PHE A | 81155.344 | 4.297 | 1.983 | 1.00 | 0.00 H |
| ATOM | 1173 | N | VAL A | 82150.265 | 1.454 | -3.713 | 1.00 | 0.00 N |
| ATOM | 1174 | CA | VAL A | 82149.439 | 1.238 | -4.894 | 1.00 | 0.00 C |
| ATOM | 1175 | C | VAL A | 82148.475 | 2.400 | -5.112 | 1.00 | 0.00 C |
| ATOM | 1176 | O | VAL A | 82148.288 | 3.238 | -4.230 | 1.00 | 0.00 O |
| ATOM | 1177 | CB | VAL A | 82148.632 | -0.069 | -4.784 | 1.00 | 0.00 C |
| ATOM | 1178 | CG1 | VAL A | 82149.555 | -1.276 | -4.862 | 1.00 | 0.00 C |
| ATOM | 1179 | CG2 | VALA | 82147.821 | -0.090 | -3.498 | 1.00 | 0.00 C |
| ATOM | 1180 | Н | VAL A | 82149.925 | 2.020 | -2.988 | 1.00 | 0.00 H |
| ATOM | 1181 | HA | VAL A | 82150.095 | 1.161 | -5.750 | 1.00 | 0.00 H |
| ATOM | 1182 | НВ | VAL A | 82147.946 | -0.116 | -5.618 | 1.00 | 0.00 H |
| ATOM | 1183 | 1HG1 | VAL A | 82150.262 | -1.240 | -4.048 | 1.00 | 0.00 H |
| ATOM | 1184 | 2HG1 | VAL A | 82150.086 | -1.262 | -5.802 | 1.00 | 0.00 H |
| ATOM | 1185 | 3HG1 | VAL A | 82148.970 | -2.181 | -4.792 | 1.00 | 0.00 H |
| ATOM | 1186 | 1HG2 | VAL A | 82147.469 | 0.907 | -3.279 | 1.00 | 0.00 H |
| ATOM | 1187 | 2HG2 | VAL A | 82148.442 | -0.439 | -2.686 | 1.00 | 0.00 H |
| ATOM | 1188 | 3HG2 | VAL A | 82146.976 | -0.752 | -3.616 | 1.00 | 0.00 H |
| ATOM | 1189 | N | LYS A | 83147.867 | 2.443 | -6.292 | 1.00 | 0.00 N |
| ATOM | 1190 | CA | LYS A | 83146.922 | 3.502 | -6.627 | 1.00 | 0.00 C |
| ATOM | 1191 | C | LYS A | 83145.691 | 3.437 | -5.732 | 1.00 | 0.00 C |
| ATOM | 1192 | О | LYS A | 83145.092 | 2.376 | -5.556 | 1.00 | 0.00 O |
| ATOM | 1193 | CB | LYS A | 83146.505 | 3.398 | -8.096 | 1.00 | 0.00 C |
| ATOM | 1194 | CG | LYS A | 83147.637 | 3.674 | -9.071 | 1.00 | 0.00 C |

| ATOM | 1195 CD | LYS A | 83147.323 | 3.133 - | 10.456 | 1.00 | 0.00 C |
|------|----------|---------|-----------|----------|--------|------|--------|
| ATOM | 1196 CE | LYS A | 83148.071 | 3.897 - | 11.536 | 1.00 | 0.00 C |
| ATOM | 1197 NZ | LYS A | 83149.309 | 3.187 - | 11.962 | 1.00 | 0.00 N |
| ATOM | 1198 H | LYS A | 83148.058 | 1.747 | -6.955 | 1.00 | 0.00 H |
| ATOM | 1199 HA | LYS A | 83147.415 | 4.449 | -6.470 | 1.00 | 0.00 H |
| ATOM | 1200 1HB | LYS A | 83146.134 | 2.401 | -8.281 | 1.00 | 0.00 H |
| ATOM | 1201 2HB | LYS A | 83145.714 | 4.108 | -8.285 | 1.00 | 0.00 H |
| ATOM | 1202 1HG | LYS A | 83147.789 | 4.740 | -9.138 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.538 | 3.203 | -8.705 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83147.611 | 2.093 -1 | 0.500 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83146.261 | 3.221 -1 | 10.634 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83147.422 | 4.015 -1 | 2.391 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83148.339 | 4.871 -1 | 1.150 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83149.120 | 2.620 -1 | 2.814 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83149.638 | 2.556 -1 | 1.205 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83150.060 | 3.875 -1 | 2.176 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.318 | 4.580 | -5.169 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.158 | 4.661 | -4.291 | 1.00 | 0.00 C |
| ATOM | 1213 C | LEU A | 84142.865 | 4.491 | -5.082 | 1.00 | 0.00 C |
| ATOM | 1214 O | LEU A | 84141.879 | 3.961 | -4.572 | 1.00 | 0.00 O |
| ATOM | 1215 CB | LEU A | 84144.151 | 6.002 | -3.554 | 1.00 | 0.00 C |
| ATOM | 1216 CG | LEU A | 84142.910 | 6.266 | -2.698 | 1.00 | 0.00 C |
| ATOM | 1217 CD | 1 LEU A | 84142.912 | 5.375 | -1.467 | 1.00 | 0.00 C |
| ATOM | 1218 CD | 2 LEU A | 84142.843 | 7.733 | -2.298 | 1.00 | 0.00 C |
| ATOM | 1219 H | LEU A | 84145.837 | 5.392 | -5.350 | 1.00 | 0.00 H |
| ATOM | 1220 HA | LEU A | 84144.233 | 3.863 | -3.568 | 1.00 | 0.00 H |
| ATOM | 1221 1HB | LEU A | 84145.020 | 6.041 | -2.914 | 1.00 | 0.00 H |

| ATOM | 1222 2HB | LEU A | 84144.229 | 6.791 | -4.287 | 1.00 | 0.00 H |
|------|-----------|-------|-----------|---------|--------|------|--------|
| ATOM | 1223 HG | LEU A | 84142.027 | 6.036 | -3.275 | 1.00 | 0.00 H |
| ATOM | 1224 1HD1 | LEU A | 84143.333 | 4.414 | -1.719 | 1.00 | 0.00 H |
| ATOM | 1225 2HD1 | LEU A | 84141.899 | 5.244 | -1.115 | 1.00 | 0.00 H |
| ATOM | 1226 3HD1 | LEU A | 84143.505 | 5.835 | -0.689 | 1.00 | 0.00 H |
| ATOM | 1227 1HD2 | LEUA | 84142.606 | 8.332 | -3.164 | 1.00 | 0.00 H |
| ATOM | 1228 2HD2 | LEU A | 84143.798 | 8.040 | -1.898 | 1.00 | 0.00 H |
| ATOM | 1229 3HD2 | LEUA | 84142.078 | 7.866 | -1.547 | 1.00 | 0.00 H |
| ATOM | 1230 N | LYS A | 85142.879 | 4.942 | -6.332 | 1.00 | 0.00 N |
| ATOM | 1231 CA | LYS A | 85141.709 | 4.839 | -7.195 | 1.00 | 0.00 C |
| ATOM | 1232 C | LYS A | 85141.357 | 3.378 | -7.464 | 1.00 | 0.00 C |
| ATOM | 1233 O | LYS A | 85140.198 | 3.045 | -7.713 | 1.00 | 0.00 O |
| ATOM | 1234 CB | LYS A | 85141.956 | 5.567 | -8.517 | 1.00 | 0.00 C |
| ATOM | 1235 CG | LYS A | 85143.160 | 5.042 | -9.284 | 1.00 | 0.00 C |
| ATOM | 1236 CD | LYS A | 85144.320 | 6.026 | -9.247 | 1.00 | 0.00 C |
| ATOM | 1237 CE | LYS A | 85144.051 | 7.236 - | 10.128 | 1.00 | 0.00 C |
| ATOM | 1238 NZ | LYS A | 85144.712 | 7.112 - | 11.457 | 1.00 | 0.00 N |
| ATOM | 1239 H | LYS A | 85143.696 | 5.354 | -6.683 | 1.00 | 0.00 H |
| ATOM | 1240 HA | LYS A | 85140.880 | 5.308 | -6.686 | 1.00 | 0.00 H |
| ATOM | 1241 1HB | LYSA | 85141.083 | 5.459 | -9.143 | 1.00 | 0.00 H |
| ATOM | 1242 2HB | LYS A | 85142.114 | 6.616 | -8.313 | 1.00 | 0.00 H |
| ATOM | 1243 1HG | LYS A | 85143.479 | 4.111 | -8.842 | 1.00 | 0.00 H |
| ATOM | 1244 2HG | LYS A | 85142.875 | 4.876 - | 10.312 | 1.00 | 0.00 H |
| ATOM | 1245 1HD | LYS A | 85144.464 | 6.360 | -8.231 | 1.00 | 0.00 H |
| ATOM | 1246 2HD | LYS A | 85145.212 | 5.528 | -9.596 | 1.00 | 0.00 H |
| ATOM | 1247 1HE | LYS A | 85142.985 | 7.331 - | 10.273 | 1.00 | 0.00 H |
| ATOM | 1248 2HE | LYS A | 85144.426 | 8.119 | -9.630 | 1.00 | 0.00 H |

| ATOM | 1249 1 | ΙHΖ | LYS A | 85145.717 | 6.869 - | 11.335 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|---------|---------|------|--------|
| ATOM | 1250 2 | 2HZ | LYS A | 85144.645 | 8.011 - | 11.975 | 1.00 | 0.00 H |
| ATOM | 1251 3 | BHZ | LYS A | 85144.251 | 6.367 - | 12.017 | 1.00 | 0.00 H |
| ATOM | 1252 | N | SER A | 86142.363 | `2.511 | -7.412 | 1.00 | 0.00 N |
| ATOM | 1253 | CA | SER A | 86142.158 | 1.087 | -7.651 | 1.00 | 0.00 C |
| ATOM | 1254 | C | SER A | 86142.188 | 0.306 | -6.341 | 1.00 | 0.00 C |
| ATOM | 1255 | О | SER A | 86142.608 | -0.850 | -6.306 | 1.00 | 0.00 O |
| ATOM | 1256 | СВ | SER A | 86143.227 | 0.549 | -8.603 | 1.00 | 0.00 C |
| ATOM | 1257 | OG | SER A | 86143.165 | 1.200 | -9.861 | 1.00 | 0.00 O |
| ATOM | 1258 | Н | SER A | 86143.265 | 2.837 | -7.209 | 1.00 | 0.00 H |
| ATOM | 1259 | НА | SER A | 86141.187 | 0.965 | -8.107 | 1.00 | 0.00 H |
| ATOM | 1260 1 | НВ | SER A | 86144.204 | 0.714 | -8.176 | 1.00 | 0.00 H |
| ATOM | 1261 2 | 2HB | SER A | 86143.073 | -0.510 | -8.752 | 1.00 | 0.00 H |
| ATOM | 1262 | HG | SER A | 86142.249 | 1.269 | -10.141 | 1.00 | 0.00 H |
| ATOM | 1263 | N | CYS A | 87141.740 | 0.946 | -5.266 | 1.00 | 0.00 N |
| ATOM | 1264 | CA | CYS A | 87141.714 | 0.312 | -3.953 | 1.00 | 0.00 C |
| ATOM | 1265 | C | CYS A | 87140.288 | -0.056 | -3.555 | 1.00 | 0.00 C |
| ATOM | 1266 | O | CYS A | 87139.363 | 0.738 | -3.721 | 1.00 | 0.00 O |
| ATOM | 1267 | СВ | CYS A | 87142.326 | 1.241 | -2.903 | 1.00 | 0.00 C |
| ATOM | 1268 | SG | CYS A | 87144.133 | 1.202 | -2.848 | 1.00 | 0.00 S |
| ATOM | 1269 | Н | CYS A | 87141.417 | 1.868 | -5.358 | 1.00 | 0.00 H |
| ATOM | 1270 | НА | CYS A | 87142.303 | -0.591 | -4.011 | 1.00 | 0.00 H |
| ATOM | 1271 | 1HB | CYS A | 87142.027 | 2.256 | -3.113 | 1.00 | 0.00 H |
| ATOM | 1272 2 | 2HB | CYS A | 87141.961 | 0.958 | -1.927 | 1.00 | 0.00 H |
| ATOM | 1273 | HG | CYS A | 87144.438 | 0.603 | -3.533 | 1.00 | 0.00 H |
| ATOM | 1274 | N | ARG A | 88140.119 | -1.265 | -3.030 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.806 | -1.737 | -2.610 | 1.00 | 0.00 C |

| ATOM | 1276 | C | ARG A | 88138.683 | -1.722 | -1.085 | 1.00 | 0.00 C |
|------|------|------|---------|-----------|--------|--------|------|--------|
| ATOM | 1277 | O | ARG A | 88139.522 | -2.287 | -0.385 | 1.00 | 0.00 O |
| ATOM | 1278 | СВ | ARG A | 88138.558 | -3.152 | -3.140 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88137.514 | -3.212 | -4.244 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88136.107 | -3.286 | -3.675 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.160 | -3.860 | -4.628 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88133.845 | -3.915 | -4.425 | 1.00 | 0.00 C |
| ATOM | 1283 | NHI | ARG A | 88133.319 | -3.434 | -3.305 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | 2 ARG A | 88133.055 | -4.454 | -5.343 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.895 | -1.853 | -2.924 | 1.00 | 0.00 H |
| ATOM | 1286 | НА | ARG A | 88138.067 | -1.072 | -3.029 | 1.00 | 0.00 H |
| ATOM | 1287 | 1HB | ARG A | 88139.485 | -3.544 | -3.530 | 1.00 | 0.00 H |
| ATOM | 1288 | 2HB | ARG A | 88138.226 | -3.779 | -2.326 | 1.00 | 0.00 H |
| ATOM | 1289 | 1HG | ARG A | 88137.598 | -2.327 | -4.856 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88137.695 | -4.089 | -4.849 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88136.123 | -3.898 | -2.786 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.784 | -2.288 | -3.417 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88135.522 | -4.222 | -5.463 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88133.909 | -3.027 | -2.609 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88132.330 | -3.480 | -3.158 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88133.446 | -4.818 | -6.189 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88132.067 | -4.496 | -5.191 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.633 | -1.072 | -0.548 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89137.417 | -0.994 | 0.901 | 1.00 | 0.00 C |
| ATOM | 1300 | C | PRO A | 89137.404 | -2.369 | 1.559 | 1.00 | 0.00 C |
| ATOM | 1301 | O | PRO A | 89136.670 | -3.264 | 1.136 | 1.00 | 0.00 O |
| ATOM | 1302 | СВ | PRO A | 89136.041 | -0.332 | 1.024 | 1.00 | 0.00 C |

| ATOM | 1303 | CG | PRO A | 89135.870 | 0.429 | -0.245 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1304 | CD | PRO A | 89136.580 | -0.368 | -1.303 | 1.00 | 0.00 C |
| ATOM | 1305 | НА | PRO A | 89138.161 | -0.375 | 1.379 | 1.00 | 0.00 H |
| ATOM | 1306 1 | HВ | PRO A | 89135.282 | -1.091 | 1.136 | 1.00 | 0.00 H |
| ATOM | 1307 2 | 2HB | PRO A | 89136.031 | 0.326 | 1.881 | 1.00 | 0.00 H |
| ATOM | 1308 1 | HG | PRO A | 89134.819 | 0.515 | -0.482 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89136.316 | 1.408 | -0.150 | 1.00 | 0.00 H |
| ATOM | 1310 1 | HD | PRO A | 89135.902 | -1.070 | -1.765 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89137.011 | 0.289 | -2.044 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASPA | 90138.220 | -2.533 | 2.594 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASP A | 90138.302 | -3.801 | 3.309 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.533 | -3.735 | 4.624 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASPA | 90138.011 | -3.166 | 5.606 | 1.00 | O.00 O |
| ATOM | 1316 | СВ | ASPA | 90139.763 | -4.165 | 3.578 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90139.987 | -5.664 | 3.624 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASPA | 90140.017 | -6.226 | 4.739 | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | ASPA | 90140.130 | -6.275 | 2.544 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.781 | -1.783 | 2.885 | 1.00 | 0.00 H |
| ATOM | 1321 | НА | ASPA | 90137.860 | -4.562 | 2.685 | 1.00 | 0.00 H |
| ATOM | 1322 1 | lНВ | ASPA | 90140.381 | -3.751 | 2.796 | 1.00 | 0.00 H |
| ATOM | 1323 2 | 2HB | ASPA | 90140.063 | -3.746 | 4.527 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.339 | -4.319 | 4.637 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91135.506 | -4.326 | 5.834 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91135.639 | -5.649 | 6.582 | 1.00 | 0.00 C |
| ATOM | 1327 | О | SER A | 91134.700 | -6.099 | 7.237 | 1.00 | 0.00 O |
| ATOM | 1328 | СВ | SER A | 91134.042 | -4.084 | 5.463 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91133.352 | -3.424 | 6.510 | 1.00 | 0.00 O |

| ATOM | 1330 | Н | SER A | 91136.012 | -4.757 | 3.824 | 1.00 | 0.00 H |
|------|--------|------|-------|-------------|---------|-------|------|--------|
| ATOM | 1331 | НА | SER A | 91135.842 | -3.527 | 6.476 | 1.00 | 0.00 H |
| ATOM | 1332 1 | НВ | SER A | 91133.994 | -3.472 | 4.575 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91133.560 | -5.032 | 5.272 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91133.254 | -4.021 | 7.255 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92136.812 | -6.266 | 6.479 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92137.067 | -7.537 | 7.147 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92137.066 | -7.367 | 8.663 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92136.736 | -8.295 | 9.401 | 1.00 | 0.00 O |
| ATOM | 1339 | CB | ARG A | 92138.406 | -8.118 | 6.689 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92138.307 | -8.944 | 5.417 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92137.309 | -10.081 | 5.568 | 1.00 | 0.00 C |
| ATOM | 1342 | NE | ARG A | 92136.010 | -9.750 | 4.987 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92134.911 | -10.481 | 5.164 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92134.949 | -11.582 | 5.903 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92133.771 - | -10.109 | 4.598 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92137.522 | -5.857 | 5.942 | 1.00 | 0.00 H |
| ATOM | 1347 | НА | ARG A | 92136.276 | -8.219 | 6.873 | 1.00 | 0.00 H |
| ATOM | 1348 1 | НВ | ARG A | 92139.095 | -7.305 | 6.511 | 1.00 | 0.00 H |
| ATOM | 1349 2 | 2HB | ARG A | 92138.800 | -8.748 | 7.472 | 1.00 | 0.00 H |
| ATOM | 1350 1 | HG | ARG A | 92137.988 | -8.305 | 4.607 | 1.00 | 0.00 H |
| ATOM | 1351 2 | 2HG | ARG A | 92139.279 | -9.357 | 5.191 | 1.00 | 0.00 H |
| ATOM | 1352 1 | HD | ĄRG A | 92137.701 | -10.956 | 5.072 | 1.00 | 0.00 H |
| ATOM | 1353 2 | 2HD | ARG A | 92137.180 | -10.293 | 6.619 | 1.00 | 0.00 H |
| ATOM | 1354 | HE | ARG A | 92135.953 | -8.941 | 4.437 | 1.00 | 0.00 H |
| ATOM | 1355 | HH1. | ARG A | 92135.807 - | 11.868 | 6.332 | 1.00 | 0.00 H |
| ATOM | 1356 2 | 2HH1 | ARG A | 92134.121 - | 12.127 | 6.032 | 1.00 | 0.00 H |

| ATOM | 1357 | HH2 | ARG A | 92133.736 | -9.280 | 4.040 | 1.00 | 0.00 H |
|------|--------|------------------|-------|-------------|----------------|--------|------|--------|
| ATOM | 1358 2 | 2HH2 | ARG A | 92132.945 - | 10.658 | 4.730 | 1.00 | 0.00 H |
| ATOM | 1359 | N | PHE A | 93137.439 | -6.176 | 9.122 | 1.00 | 0.00 N |
| ATOM | 1360 | CA | PHE A | 93137.481 | -5.887 | 10.550 | 1.00 | 0.00 C |
| ATOM | 1361 | \mathbf{C}^{-} | PHE A | 93136.780 | -4.569 | 10.863 | 1.00 | 0.00 C |
| ATOM | 1362 | О | PHE A | 93137.137 | -3.875 | 11.815 | 1.00 | 0.00 O |
| ATOM | 1363 | СВ | PHE A | 93138.930 | -5.835 | 11.037 | 1.00 | 0.00 C |
| ATOM | 1364 | CG | PHE A | 93139.691 | -7.106 | 10.797 | 1.00 | 0.00 C |
| ATOM | 1365 | CD1 | PHE A | 93140.083 | -7.907 | 11.858 | 1.00 | 0.00 C |
| ATOM | 1366 | CD2 | PHE A | 93140.013 | -7.503 | 9.508 | 1.00 | 0.00 C |
| ATOM | 1367 | CE1 | PHE A | 93140.783 | -9.078 | 11.639 | 1.00 | 0.00 C |
| ATOM | 1368 | CE2 | PHE A | 93140.713 | -8.673 | 9.283 | 1.00 | 0.00 C |
| ATOM | 1369 | CZ | PHE A | 93141.098 | - 9.462 | 10.350 | 1.00 | 0.00 C |
| ATOM | 1370 | Н | PHE A | 93137.693 | -5.476 | 8.484 | 1.00 | 0.00 H |
| ATOM | 1371 | HA | PHE A | 93136.968 | -6.685 | 11.065 | 1.00 | 0.00 H |
| ATOM | 1372 | lНВ | PHE A | 93139.446 | -5.036 | 10.524 | 1.00 | 0.00 H |
| ATOM | 1373 | 2HB | PHE A | 93138.938 | -5.637 | 12.100 | 1.00 | 0.00 H |
| ATOM | 1374 | HD1 | PHE A | 93139.836 | -7.607 | 12.866 | 1.00 | 0.00 H |
| ATOM | 1375 | HD2 | PHE A | 93139.713 | -6.887 | 8.674 | 1.00 | 0.00 H |
| ATOM | 1376 | HE1 | PHE A | 93141.083 | -9.693 | 12.475 | 1.00 | 0.00 H |
| ATOM | 1377 | HE2 | PHE A | 93140.959 | -8.971 | 8.275 | 1.00 | 0.00 H |
| ATOM | 1378 | HZ | PHE A | 93141.645 | -10.376 | 10.176 | 1.00 | 0.00 H |
| ATOM | 1379 | N | ALA A | 94135.778 | -4.230 | 10.057 | 1.00 | 0.00 N |
| ATOM | 1380 | CA | ALA A | 94135.027 | -2.996 | 10.252 | 1.00 | 0.00 C |
| ATOM | 1381 | C | ALA A | 94133.691 | -3.270 | 10.933 | 1.00 | 0.00 C |
| ATOM | 1382 | О | ALA A | 94132.872 | -4.038 | 10.431 | 1.00 | 0.00 O |
| ATOM | 1383 | СВ | ALA A | 94134.809 | -2.296 | 8.918 | 1.00 | 0.00 C |

| ATOM | 1384 | Н | ALA A | 94135.538 | -4.825 | 9.315 | 1.00 | 0.00 H |
|------|------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1385 | НА | ALA A | 94135.614 | -2.345 | 10.882 | 1.00 | 0.00 H |
| ATOM | 1386 | 1HB | ALA A | 94134.850 | -3.021 | 8.120 | 1.00 | 0.00 H |
| ATOM | 1387 | 2HB | ALA A | 94135.580 | -1.554 | 8.772 | 1.00 | 0.00 H |
| ATOM | 1388 | 3НВ | ALA A | 94133.842 | -1.815 | 8.918 | 1.00 | 0.00 H |
| ATOM | 1389 | N | SER A | 95133.478 | -2.635 | 12.081 | 1.00 | 0.00 N |
| ATOM | 1390 | CA | SER A | 95132.240 | -2.810 | 12.832 | 1.00 | 0.00 C |
| ATOM | 1391 | C | SER A | 95131.059 | -2.200 | 12.085 | 1.00 | 0.00 C |
| ATOM | 1392 | О | SER A | 95131.135 | -1.074 | 11.594 | 1.00 | 0.00 O |
| ATOM | 1393 | CB | SER A | 95132.365 | -2.173 | 14.217 | 1.00 | 0.00 C |
| ATOM | 1394 | OG | SER A | 95131.405 | -2.708 | 15.114 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95134.169 | -2.034 | 12.431 | 1.00 | 0.00 H |
| ATOM | 1396 | HA | SER A | 95132.070 | -3.870 | 12.947 | 1.00 | 0.00 H |
| ATOM | 1397 | 1HB | SER A | 95133.352 | -2.365 | 14.611 | 1.00 | 0.00 H |
| ATOM | 1398 | 2HB | SER A | 95132.210 | -1.108 | 14.137 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95130.544 | -2.721 | 14.690 | 1.00 | 0.00 H |
| ATOM | 1400 | N | LEU A | 96129.965 | -2.952 | 12.003 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96128.767 | -2.486 | 11.316 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96127.508 | -2.961 | 12.035 | 1.00 | 0.00 C |
| ATOM | 1403 | О | LEU A | 96127.307 | -4.159 | 12.230 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96128.759 | -2.981 | 9.868 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96129.541 | -2.112 | 8.882 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96129.667 | -2.811 | 7.537 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96128.869 | -0.757 | 8.719 | 1.00 | 0.00 C |
| ATOM | 1408 | Н | LEU A | 96129.965 | -3.841 | 12.415 | 1.00 | 0.00 H |
| ATOM | 1409 | HA | LEU A | 96128.783 | -1.407 | 11.317 | 1.00 | 0.00 H |
| ATOM | 1410 | 1HB | LEU A | 96129.176 | -3.978 | 9.849 | 1.00 | 0.00 H |

| ATOM | 1411 | 2HB | LEU A | 96127.733 | -3.033 | 9.534 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1412 | HG | LEU A | 96130.537 | -1.949 | 9.267 | 1.00 | 0.00 H |
| ATOM | 1413 | 1HD1 | LEU A | 96128.875 | -2.478 | 6.882 | 1.00 | 0.00 H |
| ATOM | 1414 | 2HD1 | LEU A | 96129.590 | -3.880 | 7.679 | 1.00 | 0.00 H |
| ATOM | 1415 | 3HD1 | LEU A | 96130.623 | -2.574 | 7.096 | 1.00 | 0.00 H |
| ATOM | 1416 | 1HD2 | LEU A | 96128.830 | -0.257 | 9.676 | 1.00 | 0.00 H |
| ATOM | 1417 | 2HD2 | LEU A | 96127.866 | -0.895 | 8.344 | 1.00 | 0.00 H |
| ATOM | 1418 | 3HD2 | LEU A | 96129.435 | -0.156 | 8.022 | 1.00 | 0.00 H |
| ATOM | 1419 | N | GLN A | 97126.665 | -2.011 | 12.428 | 1.00 | 0.00 N |
| ATOM | 1420 | CA | GLN A | 97125.425 | -2.332 | 13.127 | 1.00 | 0.00 C |
| ATOM | 1421 | C | GLN A | 97124.243 | -2.354 | 12.156 | 1.00 | 0.00 C |
| ATOM | 1422 | Ο | GLN A | 97123.755 | -1.304 | 11.739 | 1.00 | 0.00 O |
| ATOM | 1423 | CB | GLN A | 97125.167 | -1.315 | 14.240 | 1.00 | 0.00 C |
| ATOM | 1424 | CG | GLN A | 97125.424 | -1.863 | 15.634 | 1.00 | 0.00 C |
| ATOM | 1425 | CD | GLN A | 97124.146 | -2.256 | 16.350 | 1.00 | 0.00 C |
| ATOM | 1426 | OE1 | GLN A | 97123.962 | -1.951 | 17.528 | 1.00 | 0.00 O |
| ATOM | 1427 | NE2 | GLN A | 97123.255 | -2.938 | 15.639 | 1.00 | 0.00 N |
| ATOM | 1428 | Н | GLN A | 97126.881 | -1.073 | 12.244 | 1.00 | 0.00 H |
| ATOM | 1429 | HA | GLN A | 97125.537 | -3.311 | 13.565 | 1.00 | 0.00 H |
| ATOM | 1430 | 1HB | GLN A | 97125.810 | -0.461 | 14.089 | 1.00 | 0.00 H |
| ATOM | 1431 | 2HB | GLN A | 97124.138 | -0.993 | 14.187 | 1.00 | 0.00 H |
| ATOM | 1432 | 1HG | GLN A | 97126.055 | -2.735 | 15.554 | 1.00 | 0.00 H |
| ATOM | 1433 | 2HG | GLN A | 97125.928 | -1.107 | 16.218 | 1.00 | 0.00 H |
| ATOM | 1434 | 1HE2 | GLN A | 97123.470 | -3.146 | 14.705 | 1.00 | 0.00 H |
| ATOM | 1435 | 2HE2 | GLN A | 97122.420 | -3.205 | 16.076 | 1.00 | 0.00 H |
| ATOM | 1436 | N | PRO A | 98123.766 | -3.555 | 11.782 | 1.00 | 0.00 N |
| ATOM | 1437 | CA | PRO A | 98122.638 | -3.700 | 10.858 | 1.00 | 0.00 C |

| ATOM | 1438 | C | PRO A | 98121.303 | -3.372 | 11.518 | 1.00 | 0.00 C |
|--------|--------|-----|-------|------------|--------|--------|------|--------|
| ATOM | 1439 | О | PRO A | 98121.041 | -3.783 | 12.649 | 1.00 | 0.00 O |
| ATOM | 1440 | СВ | PRO A | 98122.694 | -5.176 | 10.467 | 1.00 | 0.00 C |
| ATOM | 1441 | CG | PRO A | 98123.315 | -5.851 | 11.641 | 1.00 | 0.00 C |
| ATOM | 1442 | CD | PRO A | 98124.286 | -4.863 | 12.229 | 1.00 | 0.00 C |
| ATOM | 1443 | НА | PRO A | 98122.765 | -3.085 | 9.979 | 1.00 | 0.00 H |
| ATOM | 1444 1 | НВ | PRO A | 98121.694 | -5.541 | 10.282 | 1.00 | 0.00 H |
| ATOM | 1445 2 | HB | PRO A | 98123.298 | -5.295 | 9.581 | 1.00 | 0.00 H |
| ATOM | 1446 1 | HG | PRO A | 98122.553 | -6.103 | 12.364 | 1.00 | 0.00 H |
| ATOM | 1447 2 | HG | PRO A | 98123.834 | -6.741 | 11.320 | 1.00 | 0.00 H |
| ATOM | 1448 1 | HD | PRO A | 98124.284 | -4.928 | 13.307 | 1.00 | 0.00 H |
| ATOM | 1449 2 | 2HD | PRO A | 98125.279 | -5.033 | 11.841 | 1.00 | 0.00 H |
| ATOM | 1450 | N | SER A | 99120.462 | -2.631 | 10.804 | 1.00 | 0.00 N |
| ATOM | 1451 | CA | SER A | 99119.153 | -2.249 | 11.322 | 1.00 | 0.00 C |
| ATOM | 1452 | C | SER A | 99118.076 | -3.219 | 10.847 | 1.00 | 0.00 C |
| ATOM | 1453 | O | SER A | 99117.225 | -3.649 | 11.627 | 1.00 | 0.00 O |
| ATOM | 1454 | CB | SER A | 99118.803 | -0.826 | 10.882 | 1.00 | 0.00 C |
| ATOM | 1455 | OG | SER A | 99117.906 | -0.216 | 11.794 | 1.00 | 0.00 O |
| ATOM | 1456 | Н | SER A | 99120.727 | -2.335 | 9.909 | 1.00 | 0.00 H |
| ATOM | 1457 | НА | SER A | 99119.200 | -2.282 | 12.399 | 1.00 | 0.00 H |
| ATOM | 1458 1 | НВ | SER A | 99119.705 | -0.235 | 10.834 | 1.00 | 0.00 H |
| ATOM | 1459 2 | 2HB | SER A | 99118.341 | -0.857 | 9.907 | 1.00 | 0.00 H |
| ATOM | 1460 | HG | SER A | 99117.119 | 0.070 | 11.326 | 1.00 | 0.00 H |
| ATOM | 1461 | N | GLY A | 100118.117 | -3.561 | 9.563 | 1.00 | 0.00 N |
| ATOM · | 1462 | CA | GLY A | 100117.140 | -4.477 | 9.006 | 1.00 | 0.00 C |
| ATOM | 1463 | C | GLY A | 100117.762 | -5.478 | 8.050 | 1.00 | 0.00 C |
| ATOM | 1464 | O | GLY A | 100118.930 | -5.840 | 8.200 | 1.00 | 0.00 O |

| ATOM | 1465 H | GLY A 100118.819 | -3.187 | 8.988 | 1.00 | 0.00 H |
|------|----------|------------------|--------|-------|------|--------|
| ATOM | 1466 1HA | GLY A 100116.667 | -5.015 | 9.815 | 1.00 | 0.00 H |
| ATOM | 1467 2HA | GLY A 100116.390 | -3.909 | 8.478 | 1.00 | 0.00 H |
| ATOM | 1468 N | PRO A 101117.001 | -5.947 | 7.047 | 1.00 | 0.00 N |
| ATOM | 1469 CA | PRO A 101117.498 | -6.916 | 6.065 | 1.00 | 0.00 C |
| ATOM | 1470 C | PRO A 101118.546 | -6.311 | 5.135 | 1.00 | 0.00 C |
| ATOM | 1471 O | PRO A 101119.493 | -6.984 | 4.730 | 1.00 | 0.00 O |
| ATOM | 1472 CB | PRO A 101116.244 | -7.303 | 5.277 | 1.00 | 0.00 C |
| ATOM | 1473 CG | PRO A 101115.329 | -6.138 | 5.425 | 1.00 | 0.00 C |
| ATOM | 1474 CD | PRO A 101115.598 | -5.570 | 6.791 | 1.00 | 0.00 C |
| ATOM | 1475 HA | PRO A 101117.909 | -7.791 | 6.546 | 1.00 | 0.00 H |
| ATOM | 1476 1HB | PRO A 101116.503 | -7.474 | 4.243 | 1.00 | 0.00 H |
| ATOM | 1477 2HB | PRO A 101115.813 | -8.199 | 5.699 | 1.00 | 0.00 H |
| ATOM | 1478 1HG | PRO A 101115.545 | -5.402 | 4.664 | 1.00 | 0.00 H |
| ATOM | 1479 2HG | PRO A 101114.302 | -6.465 | 5.351 | 1.00 | 0.00 H |
| ATOM | 1480 1HD | PRO A 101115.482 | -4.497 | 6.784 | 1.00 | 0.00 H |
| ATOM | 1481 2HD | PRO A 101114.940 | -6.018 | 7.522 | 1.00 | 0.00 H |
| ATOM | 1482 N | SER A 102118.367 | -5.037 | 4.801 | 1.00 | 0.00 N |
| ATOM | 1483 CA | SER A 102119.297 | -4.341 | 3.919 | 1.00 | 0.00 C |
| ATOM | 1484 C | SER A 102118.912 | -2.873 | 3.773 | 1.00 | 0.00 C |
| ATOM | 1485 O | SER A 102119.748 | -1.983 | 3.931 | 1.00 | 0.00 O |
| ATOM | 1486 CB | SER A 102119.328 | -5.012 | 2.544 | 1.00 | 0.00 C |
| ATOM | 1487 OG | SER A 102118.028 | -5.404 | 2.138 | 1.00 | 0.00 O |
| ATOM | 1488 H | SER A 102117.592 | -4.554 | 5.156 | 1.00 | 0.00 H |
| ATOM | 1489 HA | SER A 102120.281 | -4.401 | 4.361 | 1.00 | 0.00 H |
| ATOM | 1490 1HB | SER A 102119.724 | -4.319 | 1.817 | 1.00 | 0.00 H |
| ATOM | 1491 2HB | SER A 102119.958 | -5.888 | 2.587 | 1.00 | 0.00 H |

ATOM 1492 HG SER A 102117.584 -4.662 1.720 1.00 0.00 H **ATOM** 1493 N SER A 103117.641 -2.626 1.00 0.00 N 3.472 **ATOM** 1494 CA SER A 103117.145 -1.265 1.00 0.00 C 3.305 **ATOM** 1495 \mathbf{C} SER A 103115.622 -1.246 3.240 1.00 0.00 C **ATOM** 1496 O SER A 103114.978 -2.295 3.195 1.00 0.00 O **ATOM** 1497 CBSER A 103117.729 -0.639 2.037 1.00 0.00 C **ATOM** 1498 OG SER A 103118.925 0.066 2.321 1.00 0.00 O **ATOM** 1499 Η SER A 103117.022 -3.378 3.359 1.00 0.00 H **ATOM** 1500 HA SER A 103117.465 -0.689 4.160 1.00 0.00 H **ATOM** 1501 1HB SER A 103117.946 -1.417 1.321 1.00 0.00 H**ATOM** 1502 2HB SER A 103117.011 0.048 1.615 1.00 0.00 H **ATOM** 1503 HG SER A 103119.621 -0.234 1.732 1.00 0.00 H **ATOM** 1504 N GLY A 104115.049 -0.046 3.236 1.00 0.00 N **ATOM** 1505 CA GLY A 104113.605 0.086 3.176 1.00 0.00 C **ATOM** 1506 C GLY A 104113.168 1.467 2.728 1.00 0.00 C **ATOM** 1507 O GLY A 104112.708 2.251 3.585 1.00 0.00 O **ATOM** 1508 OXT GLY A 104113.285 1.764 1.521 1.00 0.00 O **ATOM** 1509 H GLY A 104115.612 0.755 3.273 1.00 0.00 H **ATOM** 1510 1HA GLY A 104113.216 - 0.645 2.484 1.00 0.00 H1.00 0.00 H **ATOM** 1511 2HA GLY A 104113.196 -0.108 4.157 1512 GLY A 104 TER

Three-Dimensional Structure Coordinate Table 9

ENDMDL

0.00 N ATOM 1 N GLY A 1127.996 -5.495 4.967 1.00 ATOM 2 CA GLY A 1127.436 -4.222 5.499 1.00 0.00 C 0.00 C ATOM 3 C GLY A 1127.407 -3.121 4.459 1.00

| ATOM 4 | О | GLY A | 1126.530 | -2.258 | 4.483 | 1.00 | 0.00 O | |
|--------|-----|-------|----------|--------|--------|------|--------|--|
| ATOM 5 | 1H | GLY A | 1129.036 | -5.459 | 4.975 | 1.00 | 0.00 H | |
| ATOM 6 | 2H | GLY A | 1127.674 | -5.646 | 3.989 | 1.00 | 0.00 H | |
| ATOM 7 | 3H | GLY A | 1127.683 | -6.296 | 5.551 | 1.00 | 0.00 H | |
| ATOM 8 | 1HA | GLY A | 1126.428 | -4.402 | 5.845 | 1.00 | 0.00 H | |
| ATOM 9 | 2HA | GLY A | 1128.040 | -3.898 | 6.334 | 1.00 | 0.00 H | |
| ATOM10 | N | SER A | 2128.369 | -3.150 | 3.543 | 1.00 | 0.00 N | |
| ATOM11 | CA | SER A | 2128.452 | -2.145 | 2.488 | 1.00 | 0.00 C | |
| ATOM12 | C | SER A | 2127.262 | -2.254 | 1.539 | 1.00 | 0.00 C | |
| ATOM13 | О | SER A | 2126.460 | -1.327 | 1.425 | 1.00 | 0.00 O | |
| ATOM14 | CB | SER A | 2129.758 | -2.301 | 1.707 | 1.00 | 0.00 C | |
| ATOM15 | OG | SER A | 2130.194 | -3.649 | 1.704 | 1.00 | 0.00 O | |
| ATOM16 | Н | SER A | 2129.040 | -3.863 | 3.576 | 1.00 | 0.00 H | |
| ATOM17 | НА | SER A | 2128.436 | -1.172 | 2.956 | 1.00 | 0.00 H | |
| ATOM18 | 1HB | SER A | 2129.604 | -1.984 | 0.686 | 1.00 | 0.00 H | |
| ATOM19 | 2HB | SER A | 2130.522 | -1.688 | 2.163 | 1.00 | 0.00 H | |
| ATOM20 | HG | SER A | 2130.040 | -4.034 | 0.839 | 1.00 | 0.00 H | |
| ATOM21 | N | SER A | 3127.155 | -3.392 | 0.861 | 1.00 | 0.00 N | |
| ATOM22 | CA | SER A | 3126.063 | -3.622 | -0.079 | 1.00 | 0.00 C | |
| ATOM23 | C | SER A | 3124.712 | -3.534 | 0.624 | 1.00 | 0.00 C | |
| ATOM24 | O | SER A | 3124.618 | -3.732 | 1.836 | 1.00 | 0.00 O | |
| ATOM25 | СВ | SER A | 3126.216 | -4.989 | -0.747 | 1.00 | 0.00 C | |
| ATOM26 | OG | SER A | 3126.958 | -4.889 | -1.950 | 1.00 | 0.00 O | |
| ATOM27 | Н | SER A | 3127.825 | -4.094 | 0.995 | 1.00 | 0.00 H | |
| ATOM28 | HA | SER A | 3126.111 | -2.853 | -0.836 | 1.00 | 0.00 H | |
| ATOM29 | 1HB | SER A | 3126.733 | -5.659 | -0.076 | 1.00 | 0.00 H | |
| ATOM30 | 2HB | SER A | 3125.239 | -5.388 | -0.972 | 1.00 | 0.00 H | |

| ATOM31 | HG | SER A | 3127.724 | -4.327 | -1.809 | 1.00 | 0.00 H |
|--------|-----|-------|----------|--------|--------|------|--------|
| ATOM32 | N | GLY A | 4123.668 | -3.236 | -0.143 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4122.338 | -3.127 | 0.425 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4122.252 | -2.063 | 1.500 | 1.00 | 0.00 C |
| ATOM35 | О | GLY A | 4123.271 | -1.522 | 1.928 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4123.804 | -3.088 | -1.103 | 1.00 | 0.00 H |
| ATOM37 | lHA | GLY A | 4121.641 | -2.885 | -0.364 | 1.00 | 0.00 H |
| ATOM38 | 2HA | GLY A | 4122.062 | -4.080 | 0.853 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5121.032 | -1.761 | 1.938 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5120.812 | -0.752 | 2.971 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5121.111 | 0.647 | 2.440 | 1.00 | 0.00 C |
| ATOM42 | O | SER A | 5120.218 | 1.488 | 2.344 | 1.00 | 0.00 O |
| ATOM43 | СВ | SER A | 5121.680 | -1.042 | 4.198 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5120.979 | -0.763 | 5.397 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5120.260 | -2.229 | 1.555 | 1.00 | 0.00 H |
| ATOM46 | НА | SER A | 5119.773 | -0.799 | 3.259 | 1.00 | 0.00 H |
| ATOM47 | 1HB | SER A | 5121.964 | -2.085 | 4.197 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5122.568 | -0.428 | 4.162 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5120.189 | -1.306 | 5.440 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6122.373 | 0.889 | 2.097 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6122.793 | 2.186 | 1.576 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6122.700 | 3.261 | 2.653 | 1.00 | 0.00 C |
| ATOM53 | O | SER A | 6121.654 | 3.883 | 2.837 | 1.00 | 0.00 O |
| ATOM54 | CB | SER A | 6121.937 | 2.580 | 0.369 | 1.00 | 0.00 C |
| ATOM55 | OG | SER A | 6121.576 | 1.443 | -0.394 | 1.00 | 0.00 O |
| ATOM56 | Н | SER A | 6123.040 | 0.178 | 2.198 | 1.00 | 0.00 H |
| ATOM57 | HA | SER A | 6123.822 | 2.098 | 1.262 | 1.00 | 0.00 H |

| ATOM58 1 | НB | SÉR A | 6121.038 | 3.068 | 0.713 | 1.00 | 0.00 H |
|----------|------|-------|----------|-------|--------|------|--------|
| ATOM59 2 | 2HB | SER A | 6122.497 | 3.259 | -0.259 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6120.764 | 1.623 | -0.873 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7123.804 | 3.476 | 3.363 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7123.829 | 4.477 | 4.412 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7125.104 | 5.296 | 4.400 | 1.00 | 0.00 C |
| ATOM64 | O | GLY A | 7125.065 | 6.520 | 4.527 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7124.609 | 2.950 | 3.170 | 1.00 | 0.00 H |
| ATOM66 | lΗA | GLY A | 7122.986 | 5.140 | 4.283 | 1.00 | 0.00 H |
| ATOM67 2 | 2HA | GLY A | 7123.740 | 3.983 | 5.369 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8126.238 | 4.620 | 4.248 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8127.532 | 5.292 | 4.219 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8128.105 | 5.309 | 2.805 | 1.00 | 0.00 C |
| ATOM71 | O | LEU A | 8128.927 | 4.466 | 2.448 | 1.00 | 0.00 O |
| ATOM72 | СВ | LEU A | 8128.512 | 4.600 | 5.169 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8127.931 | 4.217 | 6.531 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8128.639 | 2.991 | 7.087 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8128.039 | 5.384 | 7.502 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8126.204 | 3.645 | 4.152 | 1.00 | 0.00 H |
| ATOM77 | НА | LEU A | 8127.384 | 6.310 | 4.548 | 1.00 | 0.00 H |
| ATOM78 | lНВ | LEU A | 8128.872 | 3.702 | 4.689 | 1.00 | 0.00 H |
| ATOM79 2 | 2HB | LEU A | 8129.349 | 5.261 | 5.333 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8126.885 | 3.974 | 6.415 | 1.00 | 0.00 H |
| ATOM81 | IHD1 | LEU A | 8128.427 | 2.901 | 8.143 | 1.00 | 0.00 H |
| ATOM82 | 2HD1 | LEU A | 8129.705 | 3.094 | 6.942 | 1.00 | 0.00 H |
| ATOM83 | 3HD1 | LEU A | 8128.288 | 2.108 | 6.573 | 1.00 | 0.00 H |
| ATOM84 | HD2 | LEU A | 8127.268 | 5.299 | 8.253 | 1.00 | 0.00 H |

| ATOM85 2 | HD2 | LEU A | 4 | 8127 | .917 | 6.312 | | 6.964 | 1.00 | 0.00 H | ł |
|----------|------|-------|----|------|-------|-------|----|--------|--------|--------|--------|
| ATOM86 3 | BHD2 | LEU A | 4 | 8129 | .008 | 5.368 | } | 7.978 | 1.00 | 0.00 H | ł |
| ATOM87 | N · | ALA | Α | 912 | 7.663 | 6.27 | 4 | 2.004 | 1.00 | 0.00 | N |
| ATOM88 | CA | ALA | Α. | 912 | 8.131 | 6.40 | 0 | 0.63 | 0 1.00 | 0.00 | C |
| ATOM89 | C | ALA | Α | 912 | 3.306 | 7.86 | 4 | 0.24 | 1.00 | 0.00 | С |
| ATOM90 | O | ALA | Α | 912 | 7.411 | 8.68 | 3 | 0.450 | 1.00 | 0.00 | O |
| ATOM91 | СВ | ALA | Α | 912 | 7.166 | 5.71 | 0 | -0.321 | 1.00 | 0.00 | С |
| ATOM92 | Н | ALA | Α | 912 | 7.007 | 6.91 | 7 | 2.347 | 7 1.00 | 0.00 | H |
| ATOM93 | НА | ALA | A | 912 | 9.088 | 5.90 | 13 | 0.55 | 8 1.00 | 0.00 | Н |
| ATOM94 1 | НВ | ALA | Α | 9120 | 5.500 | 6.44 | 4 | -0.753 | 1.00 | 0.00 H | ŀ |
| ATOM95 2 | 2HB | ALA | Α | 9126 | 5.588 | 4.97 | 6 | 0.222 | 1.00 | 0.00 | Н |
| ATOM96 3 | ВНВ | ALA | Α | 912 | 7.721 | 5.22 | 2 | -1.107 | 1.00 | 0.00 H | ŀ |
| ATOM97 | N | MET | Ά | 1012 | 9.464 | 8.18 | 6 | -0.326 | 5 1.00 | 0.00 | N |
| ATOM98 | CA | MET | A | 1012 | 9.755 | 9.55 | 3 | -0.74 | 5 1.00 | 0.00 | C |
| ATOM99 | C | MET | Α | 1013 | 0.359 | 9.57 | 5 | -2.148 | 1.00 | 0.00 | C |
| ATOM | 100 | О | MI | ET A | 10131 | .577 | 9 | .500 | -2.309 | 1.00 | 0.00 O |
| ATOM | 101 | СВ | M | ETA | 10130 | 0.713 | 1(| 0.218 | 0.244 | 1.00 | 0.00 C |
| ATOM | 102 | CG | M | ET A | 1013 | 0.546 | 1 | 1.726 | 0.332 | 1.00 | 0.00 C |
| ATOM | 103 | SD | M | ET A | 10132 | 2.032 | 12 | 2.556 | 0.926 | 1.00 | 0.00 S |
| ATOM | 104 | CE | M | ET A | 10132 | 2.482 | 11 | .502 | 2.302 | 1.00. | 0.00 C |
| ATOM | 105 | Н | Ml | ET A | 10130 |).137 | 7 | 7.489 | -0.466 | 1.00 | 0.00 H |
| ATOM | 106 | HA | M | ET A | 1012 | 8.826 | 10 | 0.101 | -0.756 | 1.00 | 0.00 H |
| ATOM | 107 | 1HB | MI | ETA | 10130 | .546 | 9 | .801 | 1.225 | 1.00 | 0.00 H |
| ATOM | 108 | 2HB | MI | ET A | 10131 | .728 | 10 | 800.0 | -0.059 | 1.00 | 0.00 H |
| ATOM | 109 | 1HG | MI | ET A | 10130 |).307 | 12 | 2.107 | -0.649 | 1.00 | 0.00 H |
| ATOM | 110 | 2HG | MI | ET A | 10129 | 0.733 | 11 | .945 | 1.009 | 1.00 | 0.00 H |
| ATOM | 111 | 1HE | ME | ET A | 10131 | .660 | 10 | .838 | 2.531 | 1.00 | 0.00 H |

| ATOM | 112 2HE | MET A | 10132.704 | 12.111 | 3.166 | 1.00 | 0.00 H |
|------|---------|-------|-----------|--------|----------------|------|--------|
| ATOM | 113 3HE | MET A | 10133.353 | 10.919 | 2.040 | 1.00 | 0.00 H |
| ATOM | 114 N | PRO A | 11129.510 | 9.679 | -3.186 | 1.00 | 0.00 N |
| ATOM | 115 CA | PRO A | 11129.968 | 9.712 | -4.578 | 1.00 | 0.00 C |
| ATOM | 116 C | PRO A | 11130.980 | 10.829 | -4.830 | 1.00 | 0.00 C |
| ATOM | 117 O | PRO A | 11132.013 | 10.604 | -5.461 | 1.00 | 0.00 O |
| ATOM | 118 CB | PRO A | 11128.690 | 9.958 | -5.383 | 1.00 | 0.00 C |
| ATOM | 119 CG | PRO A | 11127.575 | 9.536 | - 4.490 | 1.00 | 0.00 C |
| ATOM | 120 CD | PRO A | 11128.044 | 9.776 | -3.082 | 1.00 | 0.00 C |
| ATOM | 121 HA | PRO A | 11130.404 | 8.768 | -4.869 | 1.00 | 0.00 H |
| ATOM | 122 1HB | PRO A | 11128.619 | 11.004 | -5.640 | 1.00 | 0.00 H |
| ATOM | 123 2HB | PRO A | 11128.714 | 9.365 | -6.286 | 1.00 | 0.00 H |
| ATOM | 124 1HG | PRO A | 11126.699 | 10.131 | -4.695 | 1.00 | 0.00 H |
| ATOM | 125 2HG | PRO A | 11127.361 | 8.488 | -4.639 | 1.00 | 0.00 H |
| ATOM | 126 1HD | PRO A | 11127.745 | 10.759 | -2.747 | 1.00 | 0.00 H |
| ATOM | 127 2HD | PRO A | 11127.654 | 9.016 | -2.420 | 1.00 | 0.00 H |
| ATOM | 128 N | PRO A | 12130.705 | 12.051 | -4.336 | 1.00 | 0.00 N |
| ATOM | 129 CA | PRO A | 12131.611 | 13.191 | -4.516 | 1.00 | 0.00 C |
| ATOM | 130 C | PRO A | 12132.995 | 12.918 | -3.938 | 1.00 | 0.00 C |
| ATOM | 131 O | PRO A | 12133.971 | 13.573 | -4.303 | 1.00 | 0.00 O |
| ATOM | 132 CB | PRO A | 12130.928 | 14.329 | -3.749 | 1.00 | 0.00 C |
| ATOM | 133 CG | PRO A | 12129.499 | 13.920 | -3.643 | 1.00 | 0.00 C |
| ATOM | 134 CD | PRO A | 12129.506 | 12.421 | -3.563 | 1.00 | 0.00 C |
| ATOM | 135 HA | PRO A | 12131.705 | 13.460 | -5.558 | 1.00 | 0.00 H |
| ATOM | 136 1HB | PRO A | 12131.382 | 14.431 | -2.775 | 1.00 | 0.00 H |
| ATOM | 137 2HB | PRO A | 12131.033 | 15.251 | -4.300 | 1.00 | 0.00 H |
| ATOM | 138 1HG | PRO A | 12129.061 | 14.342 | -2.750 | 1.00 | 0.00 H |

| ATOM | 139 2HG PRO | A 12128.957 | 14.246 | -4.519 | 1.00 | 0.00 H |
|------|--------------|--------------|----------|--------|------|--------|
| ATOM | 140 1HD PRO | A 12129.593 | 12.098 | -2.536 | 1.00 | 0.00 H |
| ATOM | 141 2HD PRO | A 12128.615 | 12.015 | -4.013 | 1.00 | 0.00 H |
| ATOM | 142 N GLY | A 13133.070 | 11.946 | -3.033 | 1.00 | 0.00 N |
| ATOM | 143 CA GLY | (A 13134.339 | 11.603 | -2.418 | 1.00 | 0.00 C |
| ATOM | 144 C GLY | A 13135.224 | 10.780 - | -3.333 | 1.00 | 0.00 C |
| ATOM | 145 O GLY | A 13135.246 | 10.995 | -4.545 | 1.00 | 0.00 O |
| ATOM | 146 H GLY | A 13132.258 | 11.458 | -2.781 | 1.00 | 0.00 H |
| ATOM | 147 1HA GLY | A 13134.858 | 12.515 - | -2.158 | 1.00 | 0.00 H |
| ATOM | 148 2HA GLY | A 13134.149 | 11.040 - | 1.517 | 1.00 | 0.00 H |
| ATOM | 149 N ASN | NA 14135.956 | 9.835 | -2.753 | 1.00 | 0.00 N |
| ATOM | 150 CA ASI | NA 14136.846 | 8.976 | -3.524 | 1.00 | 0.00 C |
| ATOM | 151 C ASN | IA 14136.100 | 7.759 | -4.061 | 1.00 | 0.00 C |
| ATOM | 152 O ASN | NA 14136.231 | 7.404 | -5.232 | 1.00 | 0.00 O |
| ATOM | 153 CB AST | NA 14138.027 | 8.525 | -2.662 | 1.00 | 0.00 C |
| ATOM | 154 CG ASI | NA 14138.857 | 9.692 | -2.162 | 1.00 | 0.00 C |
| ATOM | 155 OD1 ASN | IA 14138.854 | 10.769 | -2.756 | 1.00 | 0.00 O |
| ATOM | 156 ND2 ASN | IA 14139.573 | 9.481 | -1.064 | 1.00 | 0.00 N |
| ATOM | 157 H ASN | NA 14135.895 | 9.712 | -1.782 | 1.00 | 0.00 H |
| ATOM | 158 HA AS | NA 14137.220 | 9.551 | -4.358 | 1.00 | 0.00 H |
| ATOM | 159 1HB ASN | IA 14137.653 | 7.982 | -1.806 | 1.00 | 0.00 H |
| ATOM | 160 2HB ASN | IA 14138.663 | 7.876 | -3.245 | 1.00 | 0.00 H |
| ATOM | 161 1HD2 ASN | A 14139.527 | 8.597 - | 0.644 | 1.00 | 0.00 H |
| ATOM | 162 2HD2 ASN | A 14140.120 | 10.217 | 0.719 | 1.00 | 0.00 H |
| ATOM | 163 N SER | A 15135.315 | 7.125 - | -3.196 | 1.00 | 0.00 N |
| ATOM | 164 CA SEF | RA 15134.547 | 5.947 | -3.583 | 1.00 | 0.00 C |
| ATOM | 165 C SER | A 15133.644 | 5.488 - | 2.442 | 1.00 | 0.00 C |

| ATOM | | 166 | O | SER A | 15132.494 | 5.108 | -2.662 | 1.00 | 0.00 O |
|------|---|-----|-----|-------|-----------|-------|---------|------|--------|
| ATOM | | 167 | CB | SER A | 15135.486 | 4.812 | -3.996 | 1.00 | 0.00 C |
| ATOM | | 168 | OG | SER A | 15136.245 | 4.351 | - 2.892 | 1.00 | 0.00 O |
| ATOM | | 169 | Н | SER A | 15135.251 | 7.455 | -2.275 | 1.00 | 0.00 H |
| ATOM | | 170 | HA | SER A | 15133.930 | 6.217 | -4.427 | 1.00 | 0.00 H |
| ATOM | | 171 | 1HB | SER A | 15134.904 | 3.989 | -4.385 | 1.00 | 0.00 H |
| ATOM | | 172 | 2HB | SER A | 15136.162 | 5.168 | -4.759 | 1.00 | 0.00 H |
| ATOM | | 173 | HG | SER A | 15137.023 | 4.903 | -2.786 | 1.00 | 0.00 H |
| ATOM | | 174 | N | HIS A | 16134.175 | 5.525 | -1.224 | 1.00 | 0.00 N |
| ATOM | | 175 | CA | HIS A | 16133.417 | 5.111 | -0.049 | 1.00 | 0.00 C |
| ATOM | | 176 | C | HIS A | 16133.979 | 5.757 | 1.214 | 1.00 | 0.00 C |
| ATOM | • | 177 | O, | HIS A | 16133.236 | 6.307 | 2.026 | 1.00 | 0.00 O |
| ATOM | | 178 | СВ | HIS A | 16133.435 | 3.586 | 0.086 | 1.00 | 0.00 C |
| ATOM | | 179 | CG | HIS A | 16132.079 | 2.962 | -0.010 | 1.00 | 0.00 C |
| ATOM | | 180 | ND1 | HIS A | 16131.135 | 3.053 | 0.991 | 1.00 | 0.00 N |
| ATOM | | 181 | CD2 | HIS A | 16131.507 | 2.232 | -0.998 | 1.00 | 0.00 C |
| ATOM | | 182 | CE1 | HIS A | 16130.042 | 2.407 | 0.624 | 1.00 | 0.00 C |
| ATOM | | 183 | NE2 | HIS A | 16130.242 | 1.900 | -0.578 | 1.00 | 0.00 N |
| ATOM | | 184 | Н | HIS A | 16135.097 | 5.836 | -1.113 | 1.00 | 0.00 H |
| ATOM | 1 | 185 | НА | HIS A | 16132.397 | 5.439 | -0.181 | 1.00 | 0.00 H |
| ATOM | | 186 | 1HB | HIS A | 16134.049 | 3.170 | -0.699 | 1.00 | 0.00 H |
| ATOM | | 187 | 2HB | HIS A | 16133.858 | 3.320 | 1.044 | 1.00 | 0.00 H |
| ATOM | | 188 | HD1 | HIS A | 16131.249 | 3.521 | 1.845 | 1.00 | 0.00 H |
| ATOM | | 189 | HD2 | HIS A | 16131.962 | 1.962 | -1.940 | 1.00 | 0.00 H |
| ATOM | | 190 | HE1 | HIS A | 16129.139 | 2.311 | 1.208 | 1.00 | 0.00 H |
| ATOM | | 191 | HE2 | HIS A | 16129.625 | 1.303 | -1.049 | 1.00 | 0.00 H |
| ATOM | | 192 | N | GLY A | 17135.297 | 5.683 | 1.373 | 1.00 | 0.00 N |

| ATOM | 193 | CA | GLY A | 17135.936 | 6.264 | 2.539 | 1.00 | 0.00 C |
|--------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 194 | C | GLY A | 17137.228 | 5.562 | 2.903 | 1.00 | 0.00 C |
| ATOM . | 195 | O | GLY A | 17137.354 | 5.004 | 3.994 | 1.00 | 0.00 O |
| ATOM | 196 | Н | GLY A | 17135.839 | 5.232 | 0.693 | 1.00 | 0.00 H |
| ATOM | 197 | 1HA | GLY A | 17136.149 | 7.304 | 2.339 | 1.00 | 0.00 H |
| ATOM | 198 | 2HA | GLY A | 17135.257 | 6.203 | 3.377 | 1.00 | 0.00 H |
| ATOM | 199 | N. | LEU A | 18138.193 | 5.587 | 1.989 | 1.00 | 0.00 N |
| ATOM | 200 | CA | LEU A | 18139.483 | 4.948 | 2.219 | 1.00 | 0.00 C |
| ATOM | 201 | C | LEU A | 18140.546 | 5.982 | 2.577 | 1.00 | 0.00 C |
| ATOM | 202 | O | LEU A | 18140.944 | 6.792 | 1.741 | 1.00 | 0.00 O |
| ATOM | 203 | СВ | LEU A | 18139.915 | 4.162 | 0.980 | 1.00 | 0.00 C |
| ATOM | 204 | CG | LEU A | 18138.847 | 3.235 | 0.396 | 1.00 | 0.00 C |
| ATOM | 205 | CD1 | LEU A | 18139.067 | 3.043 | -1.097 | 1.00 | 0.00 C |
| ATOM | 206 | CD2 | LEU A | 18138.857 | 1.894 | 1.114 | 1.00 | 0.00 C |
| ATOM | 207 | Н | LEU A | 18138.033 | 6.049 | 1.139 | 1.00 | 0.00 H |
| ATOM | 208 | НА | LEU A | 18139.370 | 4.264 | 3.047 | 1.00 | 0.00 H |
| ATOM | 209 | 1HB | LEU A | 18140.207 | 4.868 | 0.216 | 1.00 | 0.00 H |
| ATOM | 210 | 2HB | LEU A | 18140.775 | 3.563 | 1.240 | 1.00 | 0.00 H |
| ATOM | 211 | HG | LEU A | 18137.875 | 3.684 | 0.534 | 1.00 | 0.00 H |
| ATOM | 212 | 1HD1 | LEU A | 18138.111 | 2.991 | -1.597 | 1.00 | 0.00 H |
| ATOM | 213 | 2HD1 | LEU A | 18139.612 | 2.126 | -1.266 | 1.00 | 0.00 H |
| ATOM | 214 | 3HD1 | LEU A | 18139.632 | 3.876 | -1.488 | 1.00 | 0.00 H |
| ATOM | 215 | 1HD2 | LEU A | 18137.880 | 1.440 | 1.041 | 1.00 | 0.00 H |
| ATOM | 216 | 2HD2 | LEU A | 18139.107 | 2.045 | 2.154 | 1.00 | 0.00 H |
| ATOM | 217 | 3HD2 | LEU A | 18139.590 | 1.246 | 0.658 | 1.00 | 0.00 H |
| ATOM | 218 | N | GLU A | 19141.003 | 5.945 | 3.825 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19142.020 | 6.879 | 4.293 | 1.00 | 0.00 C |

| ATOM | 220 | C | GLU A | 19143.006 | 6.186 | 5.228 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|-------|-------|------|--------|
| ATOM | 221 | О | GLU A | 19142.874 | 4.996 | 5.513 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19141.365 | 8.062 | 5.010 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.356 | 7.647 | 6.069 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19140.441 | 8.499 | 7.320 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19139.379 | 8.824 | 7.891 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19141.570 | 8.843 | 7.730 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.647 | 5.276 | 4.445 | 1.00 | 0.00 H |
| ATOM | 228 | HA | GLU A | 19142.556 | 7.246 | 3.431 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19142.135 | 8.649 | 5.487 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19140.856 | 8.674 | 4.280 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.363 | 7.738 | 5.657 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19140.540 | 6.618 | 6.340 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20143.994 | 6.939 | 5.702 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VAL A | 20145.003 | 6.398 | 6.605 | 1.00 | 0.00 C |
| ATOM | 235 | C | VALA | 20144.363 | 5.835 | 7.870 | 1.00 | 0.00 C |
| ATOM | 236 | Ο | VAL A | 20143.408 | 6.402 | 8.400 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VALA | 20146.035 | 7.470 | 7.000 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20147.175 | 6.849 | 7.793 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VALA | 20146.563 | 8.184 | 5.765 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20144.045 | 7.882 | 5.438 | 1.00 | 0.00 H |
| ATOM | 241 | HA | VAL A | 20145.520 | 5.603 | 6.089 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.546 | 8.199 | 7.628 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VALA | 20146.826 | 6.589 | 8.781 | 1.00 | 0.00 H |
| ATOM | 244 | 2HG1 | VAL A | 20147.987 | 7.558 | 7.873 | 1.00 | 0.00 H |
| ATOM | 245 | 3HG1 | VAL A | 20147.523 | 5.960 | 7.289 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20145.905 | 9.001 | 5.513 | 1.00 | 0.00 H |

| ATOM | 247 2 | 2HG2 | VALA | 20146.608 | 7.489 | 4.939 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 248 3 | 3HG2 | VALA | 20147.552 | 8.568 | 5.965 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.897 | 4.714 | 8.348 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.365 | 4.094 | 9.547 | 1.00 | 0.00 C |
| ATOM | 251 | ·C | GLY A | 21143.362 | 2.999 | 9.237 | 1.00 | 0.00 C |
| ATOM | 252 | O | GLY A | 21143.332 | 1.968 | 9.909 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.657 | 4.307 | 7.882 | 1.00 | 0.00 H |
| ATOM | 254 | IHA | GLY A | 21145.181 | 3.670 | 10.111 | 1.00 | 0.00 H |
| ATOM | 255 2 | 2HA | GLY A | 21143.881 | 4.850 | 10.147 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.540 | 3.222 | 8.216 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.533 | 2.247 | 7.819 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22142.140 | 1.169 | 6.927 | 1.00 | 0.00 C |
| ATOM | 259 | O | SER A | 22143.184 | 1.377 | 6.308 | 1.00 | 0.00 O |
| ATOM | 260 | CB | SER A | 22140.381 | 2.940 | 7.088 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22139.915 | 4.061 | 7.820 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.615 | 4.063 | 7.719 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22141.150 | 1.782 | 8.716 | 1.00 | 0.00 H |
| ATOM | 264 | l HB | SER A | 22140.722 | 3.275 | 6.120 | 1.00 | 0.00 H |
| ATOM | 265 2 | 2HB | SER A | 22139.566 | 2.244 | 6.962 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22139.825 | 3.824 | 8.746 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.480 | 0.017 | 6.867 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.956 | -1.095 | 6.052 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.365 | -1.033 | 4.648 | 1.00 | 0.00 C |
| ATOM | 270 | O | LEU A | 23140.256 | -0.536 | 4.451 | 1.00 | 0.00 O |
| ATOM | 271 | CB | LEU A | 23141.597 | -2.428 | 6.711 | 1.00 | 0.00 C |
| ATOM | 272 | CG | LEU A | 23142.398 | -2.764 | 7.970 | 1.00 | 0.00 C |
| ATOM | 273 | CD1 | LEU A | 23141.572 | -3.626 | 8.913 | 1.00 | 0.00 C |

| ATOM | 274 | CD2 | LEU A | 23143.697 | -3.466 | 7.602 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|---------|--------|------|--------|
| ATOM | 275 | Н | LEU A | 23140.655 | -0.089 | 7.384 | 1.00 | 0.00 H |
| ATOM | 276 | НА | LEU A | 23143.031 | -1.017 | 5.981 | 1.00 | 0.00 H |
| ATOM | 277 | 1HB | LEU A | 23140.549 | -2.406 | 6.971 | 1.00 | 0.00 H |
| ATOM | 278 | 2HB | LEU A | 23141.755 | -3.216 | 5.990 | 1.00 | 0.00 H |
| ATOM | 279 | HG | LEU A | 23142.646 | -1.848 | 8.485 | 1.00 | 0.00 H |
| ATOM | 280 | 1HD1 | LEU A | 23141.798 | -4.668 | 8.739 | 1.00 | 0.00 H |
| ATOM | 281 | 2HD1 | LEU A | 23140.522 | -3.451 | 8.734 | 1.00 | 0.00 H |
| ATOM | 282 | 3HD1 | LEU A | 23141.811 | -3.372 | 9.935 | 1.00 | 0.00 H |
| ATOM | 283 | 1HD2 | LEU A | 23144.307 | -3.580 | 8.485 | 1.00 | 0.00 H |
| ATOM | 284 | 2HD2 | LEU A | 23144.230 | -2.877 | 6.870 | 1.00 | 0.00 H |
| ATOM | 285 | 3HD2 | LEU A | 23143.475 | -4.439 | 7.190 | 1.00 | 0.00 H |
| ATOM | 286 | N | ALA A | 24142.112 | -1.543 | 3.674 | 1.00 | 0.00 N |
| ATOM | 287 | CA | ALA A | 24141.663 | -1.547 | 2.287 | 1.00 | 0.00 C |
| ATOM | 288 | C | ALA A | 24142.247 | -2.733 | 1.526 | 1.00 | 0.00 C |
| ATOM | 289 | O | ALA A | 24143.268 | -3.294 | 1.920 | 1.00 | 0.00 O |
| ATOM | 290 | CB | ALA A | 24142.041 | -0.242 | 1.605 | 1.00 | 0.00 C |
| ATOM | 291 | Н | ALA A | 24142.987 | -1.926 | 3.894 | 1.00 | 0.00 H |
| ATOM | 292 | НА | ALA A | 24140.585 | -1.627 | 2.286 | 1.00 | 0.00 H |
| ATOM | 293 | 1HB | ALAA | 24143.115 | -0.194 | 1.488 | 1.00 | 0.00 H |
| ATOM | 294 | 2HB | ALA A | 24141.710 | 0.590 | 2.210 | 1.00 | 0.00 H |
| ATOM | 295 | 3HB | ALA A | 24141.571 | -0.191 | 0.635 | 1.00 | 0.00 H |
| ATOM | 296 | N | GLU A | 25141.590 | -3.108 | 0.432 | 1.00 | 0.00 N |
| ATOM | 297 | CA | GLU A | 25142.043 | -4.228 | -0.385 | 1.00 | 0.00 C |
| ATOM | 298 | C | GLU A | 25142.350 | -3.772 | -1.808 | 1.00 | 0.00 C |
| ATOM | 299 | О | GLU A | 25141.727 | -2.844 | -2.321 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25140.984 | - 5.332 | -0.407 | 1.00 | 0.00 C |

| ATOM | 301 | CG | GLU A | 25141.514 | -6.676 | -0.879 | 1.00 | 0.00 C | |
|------|-----|------|-------|-----------|--------|--------|------|--------|--|
| ATOM | 302 | CD | GLU A | 25140.504 | -7.441 | -1.711 | 1.00 | 0.00 C | |
| ATOM | 303 | OE1 | GLU A | 25140.920 | -8.347 | -2.463 | 1.00 | 0.00 O | |
| ATOM | 304 | OE2 | GLU A | 25139.298 | -7.134 | -1.611 | 1.00 | 0.00 O | |
| ATOM | 305 | Н | GLU A | 25140.781 | -2.621 | 0.169 | 1.00 | 0.00 H | |
| ATOM | 306 | НА | GLU A | 25142.947 | -4.617 | 0.058 | 1.00 | 0.00 H | |
| ATOM | 307 | 1HB | GLU A | 25140.589 | -5.454 | 0.590 | 1.00 | 0.00 H | |
| ATOM | 308 | 2HB | GLU A | 25140.184 | -5.032 | -1.068 | 1.00 | 0.00 H | |
| ATOM | 309 | 1HG | GLU A | 25142.399 | -6.511 | -1.476 | 1.00 | 0.00 H | |
| ATOM | 310 | 2HG | GLU A | 25141.771 | -7.270 | -0.013 | 1.00 | 0.00 H | |
| ATOM | 311 | N | VAL A | 26143.315 | -4.433 | -2.442 | 1.00 | 0.00 N | |
| ATOM | 312 | CA | VALA | 26143.705 | -4.095 | -3.805 | 1.00 | 0.00 C | |
| ATOM | 313 | C | VAL A | 26143.324 | -5.207 | -4.777 | 1.00 | 0.00 C | |
| ATOM | 314 | О | VAL A | 26143.308 | -6.383 | -4.414 | 1.00 | 0.00 O | |
| ATOM | 315 | CB | VALA | 26145.219 | -3.835 | -3.909 | 1.00 | 0.00 C | |
| ATOM | 316 | CG1 | VALA | 26145.574 | -3.289 | -5.284 | 1.00 | 0.00 C | |
| ATOM | 317 | CG2 | VALA | 26145.674 | -2.882 | -2.814 | 1.00 | 0.00 C | |
| ATOM | 318 | Н | VAL A | 26143.776 | -5.165 | -1.979 | 1.00 | 0.00 H | |
| ATOM | 319 | HA | VAL A | 26143.184 | -3.191 | -4.086 | 1.00 | 0.00 H | |
| ATOM | 320 | HB | VAL A | 26145.735 | -4.775 | -3.776 | 1.00 | 0.00 H | |
| ATOM | 321 | 1HG1 | VAL A | 26145.885 | -4.100 | -5.925 | 1.00 | 0.00 H | |
| ATOM | 322 | 2HG1 | VAL A | 26146.379 | -2.575 | -5.190 | 1.00 | 0.00 H | |
| ATOM | 323 | 3HG1 | VALA | 26144.710 | -2.802 | -5.712 | 1.00 | 0.00 H | |
| ATOM | 324 | 1HG2 | VALA | 26145.138 | -1.948 | -2.905 | 1.00 | 0.00 H | |
| ATOM | 325 | 2HG2 | VAL A | 26146.733 | -2.700 | -2.913 | 1.00 | 0.00 H | |
| ATOM | 326 | 3HG2 | VAL A | 26145.472 | -3.321 | -1.849 | 1.00 | 0.00 H | |
| ATOM | 327 | N | LYS A | 27143.019 | -4.827 | -6.013 | 1.00 | 0.00 N | |

| ATOM | 328 | CA | LYS A | 27142.638 | -5.792 | -7.038 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|-----------------|--------|------|--------|
| ATOM | 329 | C | LYS A | 27143.856 | -6.246 | -7.835 | 1.00 | 0.00 C |
| ATOM | 330 | О | LYS A | 27144.131 | -5.728 | -8.917 | 1.00 | 0.00 O |
| ATOM | 331 | СВ | LYS A | 27141.596 | -5.184 | -7.978 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.860 | -6.215 | -8.820 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27141.342 | -6.206 - | 10.262 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27141.289 | -7.596 - | 10.876 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27141.792 | -7.605 - | 12.277 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27143.050 | -3.875 | -6.241 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27142.208 | -6.649 | -6.542 | 1.00 | 0.00 H |
| ATOM | 338 1 | ΙНВ | LYS A | 27140.867 | -4.647 | -7.389 | 1.00 | 0.00 H |
| ATOM | 339 2 | 2HB | LYS A | 27142.089 | -4.491 | -8.645 | 1.00 | 0.00 H |
| ATOM | 340 1 | IHG | LYS A | 27141.031 | - 7.196 | -8.400 | 1.00 | 0.00 H |
| ATOM | 341 2 | 2HG | LYS A | 27139.803 | -5.993 | -8.801 | 1.00 | 0.00 H |
| ATOM | 342 1 | IHD | LYS A | 27140.712 | -5.546 - | 10.838 | 1.00 | 0.00 H |
| ATOM | 343 2 | 2HD | LYS A | 27142.362 | -5.850 - | 10.289 | 1.00 | 0.00 H |
| ATOM | 344 1 | HE | LYS A | 27141.897 | -8.262 - | 10.281 | 1.00 | 0.00 H |
| ATOM | 345 2 | 2HE | LYS A | 27140.265 | -7.940 - | 10.867 | 1.00 | 0.00 H |
| ATOM | 346 | ΙHΖ | LYS A | 27142.831 | -7.630 - | 12.284 | 1.00 | 0.00 H |
| ATOM | 347 2 | 2HZ | LYS A | 27141.475 | -6.749 - | 12.776 | 1.00 | 0.00 H |
| ATOM | 348 3 | BHZ | LYSA | 27141.431 | -8.439 - | 12.781 | 1.00 | 0.00 H |
| ATOM | 349 | N | GLU A | 28144.583 | -7.219 | -7.294 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28145.772 | -7.744 | -7.955 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.696 | -9.263 | -8.080 | 1.00 | 0.00 C |
| ATOM | 352 | О | GLU A | 28144.649 | -9.864 | -7.844 | 1.00 | 0.00 O |
| ATOM | 353 | СВ | GLU A | 28147.030 | -7.343 | -7.180 | 1.00 | 0.00 C |
| ATOM | 354 | CG | GLU A | 28148.126 | -6.764 | -8.060 | 1.00 | 0.00 C |

| ATOM | 355 | CD | GLU A | 28148.802 | -5.560 | -7.433 | 1.00 | 0.00 C |
|------|-------|-------|-------|-----------|------------|---------|------|--------|
| ATOM | 356 | OE1 | GLU A | 28149.942 | -5.707 | -6.944 | 1.00 | 0.00 O |
| ATOM | 357 | OE2 | GLU A | 28148.191 | -4.471 | -7.431 | 1.00 | 0.00 O |
| ATOM | 358 | Н | GLU A | 28144.312 | -7.593 | -6.429 | 1.00 | 0.00 H |
| ATOM | 359 | НА | GLU A | 28145.817 | -7.315 | -8.945 | 1.00 | 0.00 H |
| ATOM | 360 | 1HB | GLU A | 28146.763 | -6.603 | -6.441 | 1.00 | 0.00 H |
| ATOM | 361 2 | 2HB | GLU A | 28147.424 | -8.215 | -6.678 | 1.00 | 0.00 H |
| ATOM | 362 | IHG | GLU A | 28148.871 | -7.526 | -8.233 | 1.00 | 0.00 H |
| ATOM | 363 2 | 2HG | GLU A | 28147.693 | -6.465 | -9.003 | 1.00 | 0.00 H |
| ATOM | 364 | N | ASN A | 29146.815 | -9.877 | -8.453 | 1.00 | 0.00 N |
| ATOM | 365 | CA | ASN A | 29146.875 | -11.325 | -8.608 | 1.00 | 0.00 C |
| ATOM | 366 | C | ASN A | 29146.931 | -12.016 | -7.247 | 1.00 | 0.00 C |
| ATOM | 367 | O | ASN A | 29146.068 | -12.831 | -6.920 | 1.00 | 0.00 O |
| ATOM | 368 | CB | ASN A | 29148.093 | -11.719 | -9.448 | 1.00 | 0.00 C |
| ATOM | 369 | CG | ASN A | 29147.735 | -11.979 | -10.898 | 1.00 | 0.00 C |
| ATOM | 370 | OD1 | ASN A | 29147.584 | -13.127 - | 11.316 | 1.00 | 0.00 O |
| ATOM | 371 | ND2 | ASN A | 29147.598 | -10.910 - | 11.674 | 1.00 | 0.00 N |
| ATOM | 372 | Н | ASN A | 29147.619 | -9.344 | -8.626 | 1.00 | 0.00 H |
| ATOM | 373 | НА | ASN A | 29145.978 | -11.640 | -9.121 | 1.00 | 0.00 H |
| ATOM | 374 | IHB . | ASN A | 29148.819 | -10.921 | -9.413 | 1.00 | 0.00 H |
| ATOM | 375 2 | 2HB | ASN A | 29148.531 | -12.617 | -9.037 | 1.00 | 0.00 H |
| ATOM | 376 | 1HD2 | ASN A | 29147.734 | -10.027 -1 | 11.273 | 1.00 | 0.00 H |
| ATOM | 377 2 | 2HD2 | ASN A | 29147.368 | -11.049 -1 | 2.616 | 1.00 | 0.00 H |
| ATOM | 378 | N | PRO A | 30147.953 | -11.697 | -6.434 | 1.00 | 0.00 N |
| ATOM | 379 | CA | PRO A | 30148.120 | -12.289 | -5.105 | 1.00 | 0.00 C |
| ATOM | 380 | C | PRO A | 30147.205 | -11.646 | -4.063 | 1.00 | 0.00 C |
| ATOM | 381 | O | PRO A | 30147.389 | -10.485 | -3.701 | 1.00 | 0.00 O |

| ATOM | 382 CB | PRO A | 30149.583 -11.995 | -4.782 | 1.00 | 0.00 C |
|------|---------|-------|-------------------|--------|------|--------|
| ATOM | 383 CG | PRO A | 30149.872 -10.721 | -5.497 | 1.00 | 0.00 C |
| ATOM | 384 CD | PRO A | 30149.028 -10.735 | -6.746 | 1.00 | 0.00 C |
| ATOM | 385 HA | PRO A | 30147.959 -13.357 | -5.123 | 1.00 | 0.00 H |
| ATOM | 386 1HB | PRO A | 30149.705 -11.890 | -3.714 | 1.00 | 0.00 H |
| ATOM | 387 2HB | PRO A | 30150.205 -12.800 | -5.145 | 1.00 | 0.00 H |
| ATOM | 388 1HG | PRO A | 30149.602 -9.881 | -4.872 | 1.00 | 0.00 H |
| ATOM | 389 2HG | PRO A | 30150.920 -10.674 | -5.754 | 1.00 | 0.00 H |
| ATOM | 390 1HD | PRO A | 30148.621 -9.752 | -6.936 | 1.00 | 0.00 H |
| ATOM | 391 2HD | PRO A | 30149.612 -11.070 | -7.590 | 1.00 | 0.00 H |
| ATOM | 392 N | PRO A | 31146.201 -12.393 | -3.566 | 1.00 | 0.00 N |
| ATOM | 393 CA | PRO A | 31145.261 -11.880 | -2.562 | 1.00 | 0.00 C |
| ATOM | 394 C | PRO A | 31145.954 -11.524 | -1.252 | 1.00 | 0.00 C |
| ATOM | 395 O | PRO A | 31146.396 -12.403 | -0.513 | 1.00 | 0.00 O |
| ATOM | 396 CB | PRO A | 31144.280 -13.041 | -2.347 | 1.00 | 0.00 C |
| ATOM | 397 CG | PRO A | 31144.464 -13.934 | -3.527 | 1.00 | 0.00 C |
| ATOM | 398 CD | PRO A | 31145.900 -13.784 | -3.937 | 1.00 | 0.00 C |
| ATOM | 399 HA | PRO A | 31144.725 -11.017 | -2.930 | 1.00 | 0.00 H |
| ATOM | 400 1HB | PRO A | 31144.523 -13.553 | -1.427 | 1.00 | 0.00 H |
| ATOM | 401 2HB | PRO A | 31143.272 -12.660 | -2.297 | 1.00 | 0.00 H |
| ATOM | 402 1HG | PRO A | 31144.257 -14.958 | -3.251 | 1.00 | 0.00 H |
| ATOM | 403 2HG | PRO A | 31143.812 -13.622 | -4.330 | 1.00 | 0.00 H |
| ATOM | 404 1HD | PRO A | 31146.524 -14.474 | -3.389 | 1.00 | 0.00 H |
| ATOM | 405 2HD | PRO A | 31146.009 -13.933 | -5.000 | 1.00 | 0.00 H |
| ATOM | 406 N | PHE A | 32146.045 -10.228 | -0.969 | 1.00 | 0.00 N |
| ATOM | 407 CA | PHE A | 32146.685 -9.757 | 0.254 | 1.00 | 0.00 C |
| ATOM | 408 C | PHE A | 32145.819 -8.715 | 0.955 | 1.00 | 0.00 C |

| ATOM | 409 | O | PHE A | 32144.887 | -8.169 | 0.365 | 1.00 | 0.00 O |
|------|-------|-----|-------|-------------|---------|---------|------|--------|
| ATOM | 410 | СВ | PHE A | 32148.062 | -9.169 | -0.058 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32148.060 | -8.215 | -1.219 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.759 | -8.514 | -2.377 | 1.00 | 0.00 C |
| ATOM | 413 | CD2 | PHE A | 32147.362 | -7.020 | -1.150 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.759 | -7.640 | -3.448 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.359 | -6.142 | -2.217 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32148.059 | -6.452 | -3.368 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.674 | -9.573 | -1.596 | 1.00 | 0.00 H |
| ATOM | 418 | НА | PHE A | 32146.807 | -10.605 | 0.911 | 1.00 | 0.00 H |
| ATOM | 419 1 | НВ | PHE A | 32148.421 | -8.635 | 0.809 | 1.00 | 0.00 H |
| ATOM | 420 2 | НВ | PHE A | 32148.746 | -9.973 | -0.287 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32149.306 | -9.443 | -2.442 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32146.815 | -6.776 | -0.252 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32149.308 | -7.885 | -4.346 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32146.811 | -5.213 | - 2.153 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32148.059 | -5.767 | -4.202 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33146.135 | -8.443 | 2.217 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.387 | -7.466 | 2.999 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33146.331 | - 6.522 | 3.736 | 1.00 | 0.00 C |
| ATOM | 429 | O | TYR A | 33147.344 | -6.948 | 4.290 | 1.00 | 0.00 O |
| ATOM | 430 | CB | TYR A | 33144.472 | -8.176 | 3.999 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33143.246 | -8.794 | 3.366 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.976 | -10.149 | 3.508 | 1.00 | 0.00 C |
| ATOM | 433 | CD2 | TYR A | 33142.360 | -8.023 | 2.625 | 1.00 | 0.00 C |
| ATOM | 434 | CE1 | TYR A | 33141.857 - | 10.718 | 2.931 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33141.238 | -8.584 | 2.045 | 1.00 | 0.00 C |

| ATOM . | 436 | CZ | TYR A | 33140.992 | -9.931 | 2.200 | 1.00 | 0.00 C |
|--------|-------|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 437 | ОН | TYR A | 33139.875 | -10.494 | 1.624 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.890 | -8.911 | 2.633 | 1.00 | 0.00 H |
| ATOM | 439 | HA | TYR A | 33144.781 | -6.890 | 2.316 | 1.00 | 0.00 H |
| ATOM | 440 | lНВ | TYR A | 33145.026 | -8.963 | 4.486 | 1.00 | 0.00 H |
| ATOM | 441 2 | 2HB | TYR A | 33144.141 | -7.464 | 4.740 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33143.656 - | 10.763 | 4.081 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.556 | -6.968 | 2.505 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33141.663 - | 11.774 | 3.053 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.561 | -7.968 | 1.472 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33140.098 | -11.360 | 1.275 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.991 | -5.237 | 3.739 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.818 | -4.253 | 4.412 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34146.029 | -3.038 | 4.858 | 1.00 | 0.00 C |
| ATOM | 450 | О | GLY A | 34144.844 | -2.911 | 4.549 | 1.00 | 0.00 O |
| ATOM | 451 | Н | GLY A | 34145.172 | -4.955 | 3.281 | 1.00 | 0.00 H |
| ATOM . | 452 | lHA | GLY A | 34147.272 | -4.712 | 5.278 | 1.00 | 0.00 H |
| ATOM | 453 2 | 2HA | GLY A | 34147.599 | -3.933 | 3.737 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.687 | -2.143 | 5.588 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VAL A | 35146.038 | -0.932 | 6.079 | 1.00 | 0.00 C |
| ATOM | 456 | C | VALA | 35146.696 | 0.316 | 5.500 | 1.00 | 0.00 C |
| ATOM | 457 | O | VAL A | 35147.920 | 0.388 | 5.382 | 1.00 | 0.00 O |
| ATOM | 458 | СВ | VAL A | 35146.078 | -0.860 | 7.619 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VAL A | 35147.514 | -0.810 | 8.119 | 1.00 | 0.00 C |
| ATOM | 460 | CG2 | VAL A | 35145.288 | 0.341 | 8.119 | 1.00 | 0.00 C |
| ATOM | 461 | Н | VAL A | 35147.629 | -2.300 | 5.802 | 1.00 | 0.00 H |
| ATOM | 462 | HA | VAL A | 35145.004 | -0.959 | 5.767 | 1.00 | 0.00 H |

| ATOM | 463 | HB | VAL A | 35145.616 | -1.754 | 8.012 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|-------|------|--------|
| ATOM | 464 | 1HG1 | VALA | 35147.617 | -1.449 | 8.984 | 1.00 | 0.00 H |
| ATOM | 465 | 2HG1 | VALA | 35147.765 | 0.205 | 8.391 | 1.00 | 0.00 H |
| ATOM | 466 | 3HG1 | VALA | 35148.179 | -1.148 | 7.339 | 1.00 | 0.00 H |
| ATOM | 467 | 1HG2 | VAL A | 35144.239 | 0.197 | 7.903 | 1.00 | 0.00 H |
| ATOM | 468 | 2HG2 | VALA | 35145.637 | 1.234 | 7.622 | 1.00 | 0.00 H |
| ATOM | 469 | 3HG2 | VALA | 35145.425 | 0.444 | 9.185 | 1.00 | 0.00 H |
| ATOM | 470 | N | ILE A | 36145.876 | 1.300 | 5.143 | 1.00 | 0.00 N |
| ATOM | 471 | CA | ILE A | 36146.379 | 2.546 | 4.577 | 1.00 | 0.00 C |
| ATOM | 472 | C | ILE A | 36147.308 | 3.255 | 5.558 | 1.00 | 0.00 C |
| ATOM | 473 | О | ILE A | 36147.020 | 3.340 | 6.751 | 1.00 | 0.00 O |
| ATOM | 474 | СВ | ILE A | 36145.228 | 3.498 | 4.194 | 1.00 | 0.00 C |
| ATOM | 475 | CG1 | ILE A | 36144.210 | 2.776 | 3.308 | 1.00 | 0.00 C |
| ATOM | 476 | CG2 | ILEA | 36145.772 | 4.732 | 3.486 | 1.00 | 0.00 C |
| ATOM | 477 | CD1 | ILE A | 36143.058 | 3.654 | 2.872 | 1.00 | 0.00 C |
| ATOM | 478 | Н | ILE A | 36144.911 | 1.184 | 5.262 | 1.00 | 0.00 H |
| ATOM | 479 | НА | ILE A | 36146.934 | 2.305 | 3.681 | 1.00 | 0.00 H |
| ATOM | 480 | HB | ILE A | 36144.741 | 3.820 | 5.102 | 1.00 | 0.00 H |
| ATOM | 481 | 1HG1 | ILE A | 36144.706 | 2.416 | 2.420 | 1.00 | 0.00 H |
| ATOM | 482 | 2HG1 | ILE A | 36143.801 | 1.936 | 3.852 | 1.00 | 0.00 H |
| ATOM | 483 | 1HG2 | ILE A | 36145.242 | 5.607 | 3.832 | 1.00 | 0.00 H |
| ATOM | 484 | 2HG2 | ILE A | 36145.632 | 4.626 | 2.420 | 1.00 | 0.00 H |
| ATOM | 485 | 3HG2 | ILE A | 36146.824 | 4.838 | 3.702 | 1.00 | 0.00 H |
| ATOM | 486 | 1HD1 | ILE A | 36142.131 | 3.246 | 3.251 | 1.00 | 0.00 H |
| ATOM | 487 | 2HD1 | ILE A | 36143.021 | 3.690 | 1.794 | 1.00 | 0.00 H |
| ATOM | 488 | 3HD1 | ILE A | 36143.197 | 4.651 | 3.263 | 1.00 | 0.00 H |
| ATOM | 489 | N | ARG A | 37148.425 | 3.761 | 5.045 | 1.00 | 0.00 N |

| ATOM | 490 | CA | ARG A | 37149.398 | 4.463 | 5.876 | 1.00 | 0.00 C |
|------|-------|--------|-------|-----------|-------|--------|------|--------|
| ATOM | 491 | C | ARG A | 37149.620 | 5.885 | 5.372 | 1.00 | 0.00 C |
| ATOM | 492 | О | ARG A | 37149.301 | 6.854 | 6.060 | 1.00 | 0.00 O |
| ATOM | 493 | СВ | ARG A | 37150.725 | 3.703 | 5.895 | 1.00 | 0.00 C |
| ATOM | 494 | CG | ARG A | 37150.572 | 2.216 | 6.176 | 1.00 | 0.00 C |
| ATOM | 495 | CD | ARG A | 37150.497 | 1.937 | 7.668 | 1.00 | 0.00 C |
| ATOM | 496 | NE | ARG A | 37149.266 | 2.455 | 8.261 | 1.00 | 0.00 N |
| ATOM | 497 | CZ | ARG A | 37149.103 | 2.662 | 9.566 | 1.00 | 0.00 C |
| ATOM | 498 | NH1 | ARG A | 37150.087 | 2.396 | 10.417 | 1.00 | 0.00 N |
| ATOM | 499 | NH2 | ARG A | 37147.951 | 3.135 | 10.023 | 1.00 | 0.00 N |
| ATOM | 500 | Н | ARG A | 37148.601 | 3.660 | 4.086 | 1.00 | 0.00 H |
| ATOM | 501 | HA | ARG A | 37149.005 | 4.507 | 6.880 | 1.00 | 0.00 H |
| ATOM | 502 | lНВ | ARG A | 37151.206 | 3.817 | 4.934 | 1.00 | 0.00 H |
| ATOM | 503 2 | 2HB | ARG A | 37151.359 | 4.128 | 6.658 | 1.00 | 0.00 H |
| ATOM | 504 | IHG | ARG A | 37149.665 | 1.864 | 5.709 | 1.00 | 0.00 H |
| ATOM | 505 2 | 2HG | ARG A | 37151.421 | 1.692 | 5.762 | 1.00 | 0.00 H |
| ATOM | 506 | IHD | ARG A | 37150.539 | 0.870 | 7.824 | 1.00 | 0.00 H |
| ATOM | 507 2 | 2HD | ARG A | 37151.343 | 2.404 | 8.151 | 1.00 | 0.00 H |
| ATOM | 508 | HE | ARG A | 37148.523 | 2.659 | 7.656 | 1.00 | 0.00 H |
| ATOM | 509 | 1HH1. | ARG A | 37150.957 | 2.038 | 10.079 | 1.00 | 0.00 H |
| ATOM | 510 2 | 2HH1 . | ARG A | 37149.958 | 2.554 | 11.395 | 1.00 | 0.00 H |
| ATOM | 511 | HH2 | ARG A | 37147.206 | 3.338 | 9.387 | 1.00 | 0.00 H |
| ATOM | 512 | 2HH2 | ARG A | 37147.828 | 3.291 | 11.003 | 1.00 | 0.00 H |
| ATOM | 513 | N | TRPA | 38150.168 | 6.003 | 4.168 | 1.00 | 0.00 N |
| ATOM | 514 | CA | TRPA | 38150.433 | 7.308 | 3.573 | 1.00 | 0.00 C |
| ATOM | 515 | C | TRP A | 38149.677 | 7.472 | 2.256 | 1.00 | 0.00 C |
| ATOM | 516 | O | TRPA | 38149.724 | 6.600 | 1.389 | 1.00 | 0.00 O |

| ATOM | 517 | CB | TRP A | 38151.937 | 7.494 | 3.343 | 1.00 | 0.00 C |
|--------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 518 | CG | TRPA | 38152.271 | 8.679 | 2.486 | 1.00 | 0.00 C |
| ATOM | 519 | CD1 | TRPA | 38152.549 | 9.947 | 2.909 | 1.00 | 0.00 C |
| ATOM | 520 | CD2 | TRPA | 38152.356 | 8.706 | 1.056 | 1.00 | 0.00 C |
| ATOM | 521 | NE1 | TRP A | 38152.802 | 10.760 | 1.830 | 1.00 | 0.00 N |
| ATOM | 522 | CE2 | TRP A | 38152.689 | 10.021 | 0.681 | 1.00 | 0.00 C |
| ATOM | 523 | CE3 | TRPA | 38152.183 | 7.745 | 0.057 | 1.00 | 0.00 C |
| ATOM | 524 | CZ2 | TRP A | 38152.852 | 10.398 | -0.650 | 1.00 | 0.00 C |
| ATOM | 525 | CZ3 | TRPA | 38152.345 | 8.119 | -1.263 | 1.00 | 0.00 C |
| ATOM | 526 | CH2 | TRPA | 38152.676 | 9.435 | -1.607 | 1.00 | 0.00 C |
| ATOM | 527 | Н | TRPA | 38150.401 | 5.193 | 3.666 | 1.00 | 0.00 H |
| ATOM . | 528 | HA | TRPA | 38150.089 | 8.062 | 4.266 | 1.00 | 0.00 H |
| ATOM | 529 1 | НВ | TRPA | 38152.427 | 7.624 | 4.296 | 1.00 | 0.00 H |
| ATOM | 530 2 | 2HB | TRPA | 38152.331 | 6.611 | 2.860 | 1.00 | 0.00 H |
| ATOM | 531 | HD1 | TRPA | 38152.564 | 10.253 | 3.945 | 1.00 | 0.00 H |
| ATOM | 532 | HE1 | TRPA | 38153.026 | 11.713 | 1.876 | 1.00 | 0.00 H |
| ATOM | 533 | HE3 | TRP A | 38151.927 | 6.725 | 0.301 | 1.00 | 0.00 H |
| ATOM | 534 | HZ2 | TRPA | 38153.105 | 11.409 | -0.931 | 1.00 | H 00.0 |
| ATOM | 535 | HZ3 | TRPA | 38152.214 | 7.389 | -2.050 | 1.00 | 0.00 H |
| ATOM | 536 | HH2 | TRPA | 38152.793 | 9.683 | -2.653 | 1.00 | 0.00 H |
| ATOM | 537 | N | ILE A | 39148.993 | 8.601 | 2.114 | 1.00 | 0.00 N |
| ATOM | 538 | CA | ILE A | 39148.236 | 8.890 | 0.902 | 1.00 | 0.00 C |
| ATOM | 539 | C | ILE A | 39148.716 | 10.190 | 0.268 | 1.00 | 0.00 C |
| ATOM | 540 | O | ILE A | 39148.434 | 11.278 | 0.771 | 1.00 | 0.00 O |
| ATOM | 541 | CB | ILE A | 39146.726 | 8.999 | 1.193 | 1.00 | 0.00 C |
| ATOM | 542 | CG1 | ILE A | 39146.253 | 7.793 | 2.006 | 1.00 | 0.00 C |
| ATOM | 543 | CG2 | ILE A | 39145.943 | 9.110 | -0.106 | 1.00 | 0.00 C |

| ATON4 | 511 | CDI | II E A | 20144 921 | 7 000 | 2.482 | 1.00 | 0.00 C |
|-------|-----|------|--------|-------------|--------|----------|------|----------|
| ATOM | 544 | | ILE A | 39144.821 | 7.908 | | | |
| ATOM | 545 | Н | ILE A | 39149.002 | 9.259 | 2.839 | 1.00 | 0.00 H |
| ATOM | 546 | HA | ILE A | 39148.392 | 8.079 | 0.207 | 1.00 | 0.00 H |
| ATOM | 547 | НВ | ILE A | 39146.556 | 9.898 | 1.765 | 1.00 | 0.00 H |
| ATOM | 548 | 1HG1 | ILE A | 39146.329 | 6.904 | 1.398 | 1.00 | 0.00 H |
| ATOM | 549 | 2HG1 | ILE A | 39146.885 | 7.682 | 2.876 | 1.00 | 0.00 H |
| ATOM | 550 | 1HG2 | ILE A | 39146.511 | 8.664 | -0.909 | 1.00 | 0.00 H |
| ATOM | 551 | 2HG2 | ILE A | 39145.761 | 10.151 | -0.328 | 1.00 | 0.00 H |
| ATOM | 552 | 3HG2 | ILE A | 39145.000 | 8.593 | - 0.003 | 1.00 | 0.00 H |
| ATOM | 553 | 1HD1 | ILE A | 39144.804 | 8.363 | 3.462 | 1.00 | 0.00 H |
| ATOM | 554 | 2HD1 | ILE A | 39144.379 | 6.925 | 2.534 | 1.00 | 0.00 H |
| ATOM | 555 | 3HD1 | ILE A | 39144.261 | 8.520 | 1.790 | 1.00 | 0.00 H |
| ATOM | 556 | N | GLY A | 40149.446 | 10.073 | -0.836 | 1.00 | 0.00 N |
| ATOM | 557 | CA | GLY A | 40149.956 | 11.250 | -1.512 | 1.00 | 0.00 C |
| ATOM | 558 | C | GLY A | 40150.450 | 10.954 | -2.913 | 1.00 | 0.00 C |
| ATOM | 559 | O | GLY A | 40150.200 | 9.877 | -3.455 | 1.00 | 0.00 O |
| ATOM | 560 | Н | GLY A | 40149.644 | 9.181 | -1.192 | 1.00 | 0.00 H |
| ATOM | 561 | 1HA | GLY A | 40149.172 | 11.988 | -1.567 | 1.00 | 0.00 H |
| ATOM | 562 | 2HA | GLY A | 40150.774 | 11.655 | -0.934 | 1.00 | 0.00 H |
| ATOM | 563 | N | GLN A | 41151.151 | 11.918 | -3.503 | 1.00 | 0.00 N |
| ATOM | 564 | CA | GLN A | 41151.682 | 11.767 | -4.850 | 1.00 | 0.00 C |
| ATOM | 565 | C | GLN A | 41153.178 | 12.077 | -4.881 | 1.00 | . 0.00 C |
| ATOM | 566 | О | GLN A | 41153.587 | 13.211 | -4.627 | 1.00 | 0.00 O |
| ATOM | 567 | СВ | GLN A | 41150.936 | 12.694 | -5.810 | 1.00 | 0.00 C |
| ATOM | 568 | CG | GLN A | A 41149.424 | 12.612 | 2 -5.681 | 1.00 | 0.00 C |
| ATOM | 569 | CD | GLN A | 41148.756 | 13.969 | -5.779 | 1.00 | 0.00 C |
| ATOM | 570 | OE1 | GLN A | 41148.808 | 14.769 | -4.846 | 1.00 | 0.00 O |
| | | | | | | | | |

| ATOM | 571 | NE2 | GLN A | 41148.124 | 14.235 | -6.916 | 1.00 | 0.00 N |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 572 | Н | GLN A | 41151.313 | 12.753 | -3.019 | 1.00 | 0.00 H |
| ATOM | 573 | НА | GLN A | 41151.527 | 10.744 | -5.158 | 1.00 | 0.00 H |
| ATOM | 574 | lНВ | GLN A | 41151.236 | 13.711 | -5.614 | 1.00 | 0.00 H |
| ATOM | 575 2 | 2HB | GLN A | 41151.205 | 12.436 | -6.822 | 1.00 | 0.00 H |
| ATOM | 576 | IHG | GLN A | 41149.040 | 11.982 | -6.470 | 1.00 | 0.00 H |
| ATOM | 577 2 | 2HG | GLN A | 41149.179 | 12.175 | -4.724 | 1.00 | 0.00 H |
| ATOM | 578 | HE2 | GLN A | 41148.124 | 13.549 | -7.616 | 1.00 | 0.00 H |
| ATOM | 579 2 | 2HE2 | GLN A | 41147.685 | 15.106 | -7.009 | 1.00 | 0.00 H |
| ATOM | 580 | N | PRO A | 42154.020 | 11.075 | -5.191 | 1.00 | 0.00 N |
| ATOM | 581 | CA | PRO A | 42155.475 | 11.257 | -5.248 | 1.00 | 0.00 C |
| ATOM | 582 | C | PRO A | 42155.883 | 12.348 | -6.233 | 1.00 | 0.00 C |
| ATOM | 583 | O | PRO A | 42155.116 | 12.706 | -7.128 | 1.00 | 0.00 O |
| ATOM | 584 | СВ | PRO A | 42155.994 | 9.893 | -5.715 | 1.00 | 0.00 C |
| ATOM | 585 | CG | PRO A | 42154.914 | 8.931 | -5.358 | 1.00 | 0.00 C |
| ATOM | 586 | CD | PRO A | 42153.628 | 9.690 | -5.508 | 1.00 | 0.00 C |
| ATOM | 587 | НА | PRO A | 42155.882 | 11.485 | -4.274 | 1.00 | 0.00 H |
| ATOM | 588 | IНВ | PRO A | 42156.167 | 9.916 | -6.781 | 1.00 | 0.00 H |
| ATOM | 589 2 | 2HB | PRO A | 42156.914 | 9.659 | -5.200 | 1.00 | 0.00 H |
| ATOM | 590 | IHG | PRO A | 42154.933 | 8.088 | -6.033 | 1.00 | 0.00 H |
| ATOM | 591 2 | 2HG | PRO A | 42155.037 | 8.600 | -4.338 | 1.00 | 0.00 H |
| ATOM | 592 | IHD | PRO A | 42153.259 | 9.615 | -6.520 | 1.00 | 0.00 H |
| ATOM | 593 2 | 2HD | PRO A | 42152.890 | 9.327 | -4.806 | 1.00 | 0.00 H |
| ATOM | 594 | N | PRO A | 43157.103 | 12.891 | -6.082 | 1.00 | 0.00 N |
| ATOM | 595 | CA | PRO A | 43157.611 | 13.946 | -6.963 | 1.00 | 0.00 C |
| ATOM | 596 | C | PRO A | 43157.953 | 13.424 | -8.354 | 1.00 | 0.00 C |
| ATOM | 597 | О | PRO A | 43159.092 | 13.042 | -8.621 | 1.00 | 0.00 O |

| ATOM | 598 | CB | PRO A | 43158.874 | 14.427 | -6.250 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|----------|---------|------|--------|
| ATOM | 599 | CG | PRO A | 43159.327 | 13.252 | -5.454 | 1.00 | 0.00 C |
| ATOM | 600 | CD | PRO A | 43158.079 | 12.520 | -5.041 | 1.00 | 0.00 C |
| ATOM | 601 | НА | PRO A | 43156.908 | 14.763 | -7.049 | 1.00 | 0.00 H |
| ATOM | 602 | lНВ | PRO A | 43159.613 | 14.718 | -6.982 | 1.00 | 0.00 H |
| ATOM | 603 2 | 2HB | PRO A | 43158.636 | 15.266 | -5.615 | 1.00 | 0.00 H |
| ATOM | 604 1 | IHG | PRO A | 43159.951 | 12.615 | -6.063 | 1.00 | 0.00 H |
| ATOM | 605 2 | 2HG | PRO A | 43159.871 | 13.587 | -4.583 | 1.00 | 0.00 H |
| ATOM | 606 1 | IHD | PRO A | 43158.252 | 11.454 | -5.037 | 1.00 | 0.00 H |
| ATOM | 607 2 | 2HD | PRO A | 43157.751 | 12.855 | -4.068 | 1.00 | 0.00 H |
| ATOM | 608 | N | GLY A | 44156.960 | 13.410 | -9.236 | 1.00 | 0.00 N |
| ATOM | 609 | CA | GLY A | 44157.179 | 12.932 - | 10.588 | 1.00 | 0.00 C |
| ATOM | 610 | C | GLY A | 44155.901 | 12.471 - | 11.257 | 1.00 | 0.00 C |
| ATOM | 611 | O | GLY A | 44155.595 | 12.885 - | 12.375 | 1.00 | 0.00 O |
| ATOM | 612 | Н | GLY A | 44156.072 | 13.725 | -8.968 | 1.00 | 0.00 H |
| ATOM | 613 | ΙHΑ | GLY A | 44157.612 | 13.728 - | 11.173 | 1.00 | 0.00 H |
| ATOM | 614 2 | 2HA | GLY A | 44157.875 | 12.105 - | 10.556 | 1.00 | 0.00 H |
| ATOM | 615 | N | LEU A | 45155.154 | 11.611 - | 10.574 | 1.00 | 0.00 N |
| ATOM | 616 | CA | LEU A | 45153.902 | 11.095 - | 11.112 | 1.00 | 0.00 C |
| ATOM | 617 | C | LEU A | 45152.735 | 11.431 - | 10.190 | 1.00 | 0.00 C |
| ATOM | 618 | 0 | LEU A | 45152.647 | 10.916 | -9.076 | 1.00 | 0.00 O |
| ATOM | 619 | CB | LEU A | 45153.993 | 9.580 - | -11.306 | 1.00 | 0.00 C |
| ATOM | 620 | CG | LEU A | 45154.530 | 8.806 | -10.099 | 1.00 | 0.00 C |
| ATOM | 621 | CD1 | LEU A | 45154.083 | 7.352 - | 10.154 | 1.00 | 0.00 C |
| ATOM | 622 | CD2 | LEU A | 45156.049 | 8.900 - | 10.039 | 1.00 | 0.00 C |
| ATOM | 623 | Н | LEU A | 45155.450 | 11.319 | -9.685 | 1.00 | 0.00 H |
| ATOM | 624 | НА | LEU A | 45153.734 | 11.562 | -12.070 | 1.00 | 0.00 H |

| ATOM | 625 1HB | LEU A | 45153.006 | 9.208 -11.537 | 1.00 0.00 H |
|------|----------|---------|-----------|----------------|---------------|
| ATOM | 626 2HB | LEU A | 45154.640 | 9.384 -12.147 | 1.00 0.00 H |
| ATOM | 627 HG | LEU A | 45154.131 | 9.243 -9.196 | 5 1.00 0.00 H |
| ATOM | 628 1HD1 | LEU A | 45153.399 | 7.155 -9.341 | 1.00 0.00 H |
| ATOM | 629 2HD1 | LEU A | 45154.943 | 6.705 -10.064 | 1.00 0.00 H |
| ATOM | 630 3HD1 | LEU A | 45153.587 | 7.161 -11.094 | 1.00 0.00 H |
| ATOM | 631 1HD2 | LEU A | 45156.481 | 7.939 -10.273 | 1.00 0.00 H |
| ATOM | 632 2HD2 | LEU A | 45156.351 | 9.197 -9.044 | 1.00 0.00 H |
| ATOM | 633 3HD2 | LEU A | 45156.395 | 9.634 -10.752 | 1.00 0.00 H |
| ATOM | 634 N | ASN A | 46151.839 | 12.293 -10.660 | 1.00 0.00 N |
| ATOM | 635 CA | ASN A | 46150.682 | 12.685 -9.866 | 5 1.00 0.00 C |
| ATOM | 636 C | ASN A | 46149.666 | 11.550 -9.807 | 1.00 0.00 C |
| ATOM | 637 O | ASN A | 46148.992 | 11.253 -10.792 | 1.00 0.00 O |
| ATOM | 638 CB | ASN A | 46150.034 | 13.937 -10.460 | 1.00 0.00 C |
| ATOM | 639 CG | ASN A | 46149.364 | 14.797 -9.406 | 6 1.00 0.00 C |
| ATOM | 640 OD | I ASN A | 46149.991 | 15.199 -8.426 | 1.00 0.00 O |
| ATOM | 641 ND2 | 2 ASN A | 46148.083 | 15.083 -9.604 | 1.00 0.00 N |
| ATOM | 642 H | ASN A | 46151.958 | 12.670 -11.556 | 1.00 0.00 H |
| ATOM | 643 HA | ASN A | 46151.023 | 12.904 -8.865 | 5 1.00 0.00 H |
| ATOM | 644 1HB | ASN A | 46150.792 | 14.529 -10.950 | 1.00 0.00 H |
| ATOM | 645 2HB | ASN A | 46149.290 | 13.640 -11.184 | 1.00 0.00 H |
| ATOM | 646 1HD2 | ASN A | 46147.648 | 14.729 -10.408 | 1.00 0.00 H |
| ATOM | 647 2HD2 | ASN A | 46147.625 | 15.639 -8.939 | 1.00 0.00 H |
| ATOM | 648 N | GLU A | 47149.563 | 10.920 -8.642 | 2 1.00 0.00 N |
| ATOM | 649 CA | GLU A | 47148.631 | 9.817 -8.44 | 7 1.00 0.00 C |
| ATOM | 650 C | GLU A | 47148.480 | 9.494 -6.965 | 1.00 0.00 C |
| ATOM | 651 O | GLU A | 47149.455 | 9.161 -6.291 | 1.00 0.00 O |

| ATOM | 652 | СВ | GLU A | 47149.104 | 8.574 | -9.206 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|---------|---------|------|--------|
| ATOM | 653 | CG | GLU A | 47150.611 | 8.372 | -9.178 | 1.00 | 0.00 C |
| ATOM | 654 | CD | GLU A | 47151.090 | 7.413 | -10.250 | 1.00 | 0.00 C |
| ATOM | 655 | OE1 | GLU A | 47151.384 | 6.246 | -9.915 | 1.00 | 0.00 O |
| ATOM | 656 | OE2 | GLU A | 47151.171 | 7.829 - | -11.425 | 1.00 | 0.00 O |
| ATOM | 657 | Н | GLU A | 47150.130 | 11.205 | -7.896 | 1.00 | 0.00 H |
| ATOM | 658 | НА | GLU A | 47147.671 | 10.122 | -8.836 | 1.00 | 0.00 H |
| ATOM | 659 | 1HB | GLU A | 47148.638 | 7.703 | -8.771 | 1.00 | 0.00 H |
| ATOM | 660 | 2HB | GLU A | 47148.793 | 8.658 | -10.237 | 1.00 | 0.00 H |
| ATOM | 661 | 1HG | GLU A | 47151.093 | 9.326 | -9.329 | 1.00 | 0.00 H |
| ATOM | 662 | 2HG | GLU A | 47150.892 | 7.978 | -8.212 | 1.00 | 0.00 H |
| ATOM | 663 | N | VAL A | 48147.255 | 9.585 | -6.461 | 1.00 | 0.00 N |
| ATOM | 664 | CA | VALA | 48146.988 | 9.294 | -5.059 | 1.00 | 0.00 C |
| ATOM | 665 | C | VALA | 48147.302 | 7.836 | -4.743 | 1.00 | 0.00 C |
| ATOM | 666 | О | VAL A | 48146.505 | 6.943 | -5.029 | 1.00 | 0.00 O |
| ATOM | 667 | CB | VALA | 48145.522 | 9.585 | -4.689 | 1.00 | 0.00 C |
| ATOM | 668 | CG1 | VAL A | 48145.318 | 9.474 | -3.186 | 1.00 | 0.00 C |
| ATOM | 669 | CG2 | VALA | 48145.108 | 10.959 | -5.192 | 1.00 | 0.00 C |
| ATOM | 670 | Н | VAL A | 48146.514 | 9.850 | -7.045 | 1.00 | 0.00 H |
| ATOM | 671 | HA | VAL A | 48147.625 | 9.928 | -4.458 | 1.00 | 0.00 H |
| ATOM | 672 | HB | VAL A | 48144.897 | 8.846 | -5.169 | 1.00 | 0.00 H |
| ATOM | 673 | 1HG1 | VALA | 48145.394 | 8.440 | -2.887 | 1.00 | 0.00 H |
| ATOM | 674 | 2HG1 | VALA | 48144.339 | 9.853 | -2.928 | 1.00 | 0.00 H |
| ATOM | 675 | 3HG1 | VAL A | 48146.073 | 10.054 | -2.677 | 1.00 | 0.00 H |
| ATOM | 676 | 1HG2 | VAL A | 48144.413 | 11.403 | -4.495 | 1.00 | 0.00 H |
| ATOM | 677 | 2HG2 | VALA | 48144.636 | 10.861 | -6.158 | 1.00 | 0.00 H |
| ATOM | 678 | 3HG2 | VAL A | 48145.981 | 11.589 | -5.280 | 1.00 | 0.00 H |

| ATOM | 679 | N | LEU A | 49148.472 | 7.601 | -4.156 | 1.00 | 0.00 N |
|------|-----|------|-------|-----------|-------|---------|------|--------|
| ATOM | 680 | CA | LEU A | 49148.892 | 6.250 | - 3.807 | 1.00 | 0.00 C |
| ATOM | 681 | C | LEU A | 49148.847 | 6.042 | -2.299 | 1.00 | 0.00 C |
| ATOM | 682 | О | LEU A | 49149.562 | 6.707 | -1.549 | 1.00 | 0.00 O |
| ATOM | 683 | CB | LEU A | 49150.306 | 5.982 | -4.327 | 1.00 | 0.00 C |
| ATOM | 684 | CG | LEU A | 49150.455 | 6.034 | -5.849 | 1.00 | 0.00 C |
| ATOM | 685 | CD1 | LEU A | 49151.876 | 6.420 | -6.232 | 1.00 | 0.00 C |
| ATOM | 686 | CD2 | LEU A | 49150.080 | 4.696 | -6.467 | 1.00 | 0.00 C |
| ATOM | 687 | H | LEU A | 49149.066 | 8.354 | -3.954 | 1.00 | 0.00 H |
| ATOM | 688 | HA | LEU A | 49148.208 | 5.558 | -4.274 | 1.00 | 0.00 H |
| ATOM | 689 | 1HB | LEU A | 49150.971 | 6.715 | -3.896 | 1.00 | 0.00 H |
| ATOM | 690 | 2HB | LEU A | 49150.610 | 5.002 | -3.992 | 1.00 | 0.00 H |
| ATOM | 691 | HG | LEU A | 49149.787 | 6.786 | -6.245 | 1.00 | 0.00 H |
| ATOM | 692 | 1HD1 | LEU A | 49152.135 | 7.354 | -5.757 | 1.00 | 0.00 H |
| ATOM | 693 | 2HD1 | LEU A | 49151.942 | 6.530 | -7.304 | 1.00 | 0.00 H |
| ATOM | 694 | 3HD1 | LEU A | 49152.559 | 5.649 | -5.906 | 1.00 | 0.00 H |
| ATOM | 695 | 1HD2 | LEU A | 49149.173 | 4.330 | -6.007 | 1.00 | 0.00 H |
| ATOM | 696 | 2HD2 | LEU A | 49150.878 | 3.987 | -6.303 | 1.00 | 0.00 H |
| ATOM | 697 | 3HD2 | LEU A | 49149.920 | 4.821 | -7.527 | 1.00 | 0.00 H |
| ATOM | 698 | N | ALA A | 50148.001 | 5.118 | -1.861 | 1.00 | 0.00 N |
| ATOM | 699 | CA | ALA A | 50147.865 | 4.827 | -0.441 | 1.00 | 0.00 C |
| ATOM | 700 | C | ALA A | 50148.802 | 3.700 | -0.019 | 1.00 | 0.00 C |
| ATOM | 701 | Ο | ALA A | 50148.655 | 2.561 | -0.462 | 1.00 | 0.00 O |
| ATOM | 702 | CB | ALA A | 50146.423 | 4.471 | -0.111 | 1.00 | 0.00 C |
| ATOM | 703 | Н | ALA A | 50147.456 | 4.621 | -2.506 | 1.00 | 0.00 H |
| ATOM | 704 | HA | ALA A | 50148.124 | 5.723 | 0.106 | 1.00 | 0.00 H |
| ATOM | 705 | 1HB | ALA A | 50146.405 | 3.738 | 0.682 | 1.00 | 0.00 H |

| ATOM | 706 | 2HB | ALA A | 50145.943 | 4.063 | -0.988 | 1.00 | 0.00 H |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 707 | 3НВ | ALA A | 50145.896 | 5.358 | 0.208 | 1.00 | 0.00 H |
| ATOM | 708 | N | GLY A | 51149.764 | 4.024 | 0.838 | 1.00 | 0.00 N |
| ATOM | 709 | CA | GLY A | 51150.710 | 3.029 | 1.304 | 1.00 | 0.00 C |
| ATOM | 710 | C | GLY A | 51150.071 | 2.011 | 2.229 | 1.00 | 0.00 C |
| ATOM | 711 | O | GLY A | 51149.790 | 2.310 | 3.390 | 1.00 | 0.00 O |
| ATOM | 712 | Н | GLY A | 51149.832 | 4.950 | 1.156 | 1.00 | 0.00 H |
| ATOM | 713 | 1HA | GLY A | 51151.122 | 2.512 | 0.450 | 1.00 | 0.00 H |
| ATOM | 714 | 2HA | GLY A | 51151.510 | 3.526 | 1.830 | 1.00 | 0.00 H |
| ATOM | 715 | N | LEU A | 52149.841 | 0.808 | 1.715 | 1.00 | 0.00 N |
| ATOM | 716 | CA | LEU A | 52149.231 | -0.256 | 2.503 | 1.00 | 0.00 C |
| ATOM | 717 | C | LEU A | 52150.296 | -1.119 | 3.171 | 1.00 | 0.00 C |
| ATOM | 718 | O | LEU A | 52151.352 | -1.377 | 2.594 | 1.00 | 0.00 O |
| ATOM | 719 | CB | LEU A | 52148.333 | -1.124 | 1.619 | 1.00 | 0.00 C |
| ATOM | 720 | CG | LEU A | 52147.158 | -0.390 | 0.972 | 1.00 | 0.00 C |
| ATOM | 721 | CD1 | LEU A | 52146.581 | -1.211 | -0.171 | 1.00 | 0.00 C |
| ATOM | 722 | CD2 | LEU A | 52146.085 | -0.087 | 2.006 | 1.00 | 0.00 C |
| ATOM | 723 | Н | LEU A | 52150.088 | 0.631 | 0.782 | 1.00 | 0.00 H |
| ATOM | 724 | НА | LEU A | 52148.627 | 0.206 | 3.271 | 1.00 | 0.00 H |
| ATOM | 725 | 1HB | LEU A | 52148.942 | -1.551 | 0.835 | 1.00 | 0.00 H |
| ATOM | 726 | 2HB | LEU A | 52147.938 | -1.928 | 2.223 | 1.00 | 0.00 H |
| ATOM | 727 | HG | LEU A | 52147.507 | 0.548 | 0.565 | 1.00 | 0.00 H |
| ATOM | 728 | 1HD1 | LEU A | 52145.819 | -1.874 | 0.211 | 1.00 | 0.00 H |
| ATOM | 729 | 2HD1 | LEU A | 52147.367 | -1.793 | -0.630 | 1.00 | 0.00 H |
| ATOM | 730 | 3HD1 | LEU A | 52146.147 | -0.550 | -0.906 | 1.00 | 0.00 H |
| ATOM | 731 | 1HD2 | LEU A | 52145.114 | -0.103 | 1.534 | 1.00 | 0.00 H |
| ATOM | 732 | 2HD2 | LEU A | 52146.261 | 0.891 | 2.432 | 1.00 | 0.00 H |

| ATOM | 733 | 3HD2 | LEU A | 52146.118 | -0.831 | 2.789 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|-------|------|--------|
| ATOM | 734 | N | GLU A | 53150.010 | -1.565 | 4.390 | 1.00 | 0.00 N |
| ATOM | 735 | CA | GLU A | 53150.943 | -2.400 | 5.137 | 1.00 | 0.00 C |
| ATOM | 736 | C | GLU A | 53150.426 | -3.831 | 5.244 | 1.00 | 0.00 C |
| ATOM | 737 | O | GLU A | 53149.452 | -4.099 | 5.948 | 1.00 | 0.00 O |
| ATOM | 738 | CB | GLU A | 53151.171 | -1.823 | 6.535 | 1.00 | 0.00 C |
| ATOM | · 739 | CG | GLU A | 53152.170 | -2.613 | 7.365 | 1.00 | 0.00 C |
| ATOM | 740 | CD | GLU A | 53151.776 | -2.697 | 8.827 | 1.00 | 0.00 C |
| ATOM | 741 | OE1 | GLU A | 53152.274 | -3.607 | 9.524 | 1.00 | 0.00 O |
| ATOM | 742 | OE2 | GLU A | 53150.970 | -1.856 | 9.275 | 1.00 | 0.00 O |
| ATOM | 743 | H, | GLU A | 53149.151 | -1.326 | 4.797 | 1.00 | 0.00 H |
| ATOM | 744 | HA | GLU A | 53151.882 | -2.409 | 4.604 | 1.00 | 0.00 H |
| ATOM | 745 | 1HB | GLU A | 53151.536 | -0.811 | 6.440 | 1.00 | 0.00 H |
| ATOM | 746 | 2HB | GLU A | 53150.229 | -1.809 | 7.064 | 1.00 | 0.00 H |
| ATOM | 747 | 1HG | GLU A | 53152.236 | -3.615 | 6.968 | 1.00 | 0.00 H |
| ATOM | 748 | 2HG | GLU A | 53153.135 | -2.134 | 7.295 | 1.00 | 0.00 H |
| ATOM | 749 | N | LEU A | 54151.083 | -4.747 | 4.540 | 1.00 | 0.00 N |
| ATOM | 750 | CA | LEU A | 54150.690 | -6.152 | 4.556 | 1.00 | 0.00 C |
| ATOM | 751 | C | LEU A | 54150.936 | -6.770 | 5.929 | 1.00 | 0.00 C |
| ATOM | 752 | O | LEU A | 54151.987 | -6.563 | 6.535 | 1.00 | 0.00 O |
| ATOM | 753 | СВ | LEU A | 54151.460 | -6.929 | 3.488 | 1.00 | 0.00 C |
| ATOM | 754 | CG | LEU A | 54151.434 | -6.309 | 2.090 | 1.00 | 0.00 C |
| ATOM | 755 | CD1 | LEU A | 54152.561 | -6.869 | 1.236 | 1.00 | 0.00 C |
| ATOM | 756 | CD2 | LEUA | 54150.087 | -6.552 | 1.425 | 1.00 | 0.00 C |
| ATOM | 757 | Н | LEU A | 54151.852 | -4.472 | 3.997 | 1.00 | 0.00 H |
| ATOM | 758 | НА | LEU A | 54149.635 | -6.202 | 4.335 | 1.00 | 0.00 H |
| ATOM | 759 | 1HB | LEU A | 54152.490 | -7.011 | 3.805 | 1.00 | 0.00 H |

| ATOM | 760 2HB | LEU A | 54151.042 | -7.922 | 3.424 | 1.00 | 0.00 H | |
|------|----------|-------|-------------|---------|-------|------|--------|---|
| ATOM | 761 HG | LEU A | 54151.578 | -5.241 | 2.175 | 1.00 | 0.00 H | |
| ATOM | 762 1HD1 | LEU A | 54153.480 | -6.863 | 1.804 | 1.00 | 0.00 H | |
| ATOM | 763 2HD1 | LEU A | 54152.680 | -6.260 | 0.352 | 1.00 | 0.00 H | |
| ATOM | 764 3HD1 | LEU A | 54152.324 | -7.882 | 0.947 | 1.00 | 0.00 H | |
| ATOM | 765 1HD2 | LEU A | 54149.633 | -7.438 | 1.847 | 1.00 | 0.00 H | , |
| ATOM | 766 2HD2 | LEU A | 54150.229 | -6.692 | 0.364 | 1.00 | 0.00 H | |
| ATOM | 767 3HD2 | LEU A | 54149.443 | -5.702 | 1.595 | 1.00 | 0.00 H | |
| ATOM | 768 N | GLU A | 55149.958 | -7.528 | 6.413 | 1.00 | 0.00 N | |
| ATOM | 769 CA | GLU A | 55150.067 | -8.176 | 7.715 | 1.00 | 0.00 C | |
| ATOM | 770 C | GLU A | 55151.139 | -9.261 | 7.696 | 1.00 | 0.00 C | |
| ATOM | 771 O | GLU A | 55151.836 | -9.478 | 8.686 | 1.00 | 0.00 O | |
| ATOM | 772 CB | GLU A | 55148.722 | -8.779 | 8.123 | 1.00 | 0.00 C | |
| ATOM | 773 CG | GLU A | 55147.657 | -7.739 | 8.430 | 1.00 | 0.00 C | |
| ATOM | 774 CD | GLU A | 55146.711 | -7.512 | 7.268 | 1.00 | 0.00 C | |
| ATOM | 775 OE1 | GLU A | 55146.763 | -6.420 | 6.663 | 1.00 | 0.00 O | |
| ATOM | 776 OE2 | GLU A | 55145.916 | -8.426 | 6.962 | 1.00 | 0.00 O | |
| ATOM | 777 H | GLU A | 55149.144 | -7.655 | 5.884 | 1.00 | 0.00 H | |
| ATOM | 778 HA | GLU A | 55150.347 | -7.424 | 8.437 | 1.00 | 0.00 H | |
| ATOM | 779 1HB | GLU A | 55148.361 | -9.404 | 7.319 | 1.00 | 0.00 H | |
| ATOM | 780 2HB | GLU A | 55148.864 | -9.388 | 9.003 | 1.00 | 0.00 H | |
| ATOM | 781 1HG | GLU A | 55147.083 | -8.069 | 9.283 | 1.00 | 0.00 H | |
| ATOM | 782 2HG | GLU A | 55148.143 | -6.803 | 8.667 | 1.00 | 0.00 H | |
| ATOM | 783 N | ASP A | 56151.263 | -9.943 | 6.561 | 1.00 | 0.00 N | |
| ATOM | 784 CA | ASPA | 56152.251 - | -11.006 | 6.412 | 1.00 | 0.00 C | |
| ATOM | 785 C | ASPA | 56153.446 - | 10.528 | 5.596 | 1.00 | 0.00 C | |
| ATOM | 786 O | ASPA | 56153.285 | -9.897 | 4.551 | 1.00 | 0.00 O | |

| ATOM | 787 | CB | ASPA | 56151.617 | -12.228 | 5.745 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|---------|-------|------|--------|
| ATOM | 788 | CG | ASPA | 56151.036 | -13.201 | 6.753 | 1.00 | 0.00 C |
| ATOM | 789 | OD1 | ASP A | 56149.897 | -13.665 | 6.541 | 1.00 | 0.00 O |
| ATOM | 790 | OD2 | ASPA | 56151.722 | -13.498 | 7.754 | 1.00 | 0.00 O |
| ATOM | 791 | Н | ASPA | 56150.678 | -9.724 | 5.806 | 1.00 | 0.00 H |
| ATOM | 792 | НА | ASPA | 56152.591 | -11.281 | 7.399 | 1.00 | 0.00 H |
| ATOM | 793 1 | HB | ASPA | 56150.825 | -11.902 | 5.089 | 1.00 | 0.00 H |
| ATOM | 794 2 | HB | ASPA | 56152.370 | -12.744 | 5.167 | 1.00 | 0.00 H |
| ATOM | 795 | N | GLU A | 57154.646 | -10.834 | 6.078 | 1.00 | 0.00 N |
| ATOM | 796 | CA | GLU A | 57155.870 | -10.436 | 5.392 | 1.00 | 0.00 C |
| ATOM | 797 | C | GLU A | 57155.928 | -11.034 | 3.991 | 1.00 | 0.00 C |
| ATOM | 798 | O | GLU A | 57156.352 | -12.176 | 3.810 | 1.00 | 0.00 O |
| ATOM | 799 | CB | GLU A | 57157.095 | -10.872 | 6.197 | 1.00 | 0.00 C |
| ATOM | 800 | CG | GLU A | 57157.104 | -10.349 | 7.624 | 1.00 | 0.00 C |
| ATOM | 801 | CD | GLU A | 57156.564 | -11.358 | 8.618 | 1.00 | 0.00 C |
| ATOM | 802 | OE1 | GLU A | 57156.945 | -11.284 | 9.805 | 1.00 | 0.00 O |
| ATOM | 803 | OE2 | GLU A | 57155.759 | -12.221 | 8.210 | 1.00 | 0.00 O |
| ATOM | 804 | Н | GLU A | 57154.710 | -11.339 | 6.915 | 1.00 | 0.00 H |
| ATOM | 805 | НА | GLU A | 57155.869 | -9.359 | 5.311 | 1.00 | 0.00 H |
| ATOM | 806 1 | HB | GLU A | 57157.123 | -11.951 | 6.233 | 1.00 | 0.00 H |
| ATOM | 807 2 | HB | GLU A | 57157.985 | -10.514 | 5.700 | 1.00 | 0.00 H |
| ATOM | 808 1 | HG | GLU A | 57158.120 | -10.105 | 7.898 | 1.00 | 0.00 H |
| ATOM | 809 2 | HG | GLU A | 57156.496 | -9.458 | 7.671 | 1.00 | 0.00 H |
| ATOM | 810 | N | CYS A | 58155.499 | -10.256 | 3.003 | 1.00 | 0.00 N |
| ATOM | 811 | CA | CYS A | 58155.502 | -10.709 | 1.617 | 1.00 | 0.00 C |
| ATOM | 812 | C | CYS A | 58156.853 | -10.442 | 0.960 | 1.00 | 0.00 C |
| ATOM | 813 | O | CYS A | 58157.328 | -9.307 | 0.933 | 1.00 | 0.00 O |

| ATOM | 814 | CB | CYS A | 58154.392 | -10.013 | 0.828 | 1.00 | 0.00 C |
|--------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 815 | SG | CYS A | 58154.271 | -10.539 | -0.897 | 1.00 | 0.00 S |
| ATOM | 816 | Н | CYS A | 58155.173 | -9.355 | 3.210 | 1.00 | 0.00 H |
| ATOM | 817 | НА | CYS A | 58155.319 | -11.773 | 1.616 | 1.00 | 0.00 H |
| ATOM | 818 | 1HB | CYS A | 58153.443 - | 10.217 | 1.300 | 1.00 | 0.00 H |
| ATOM | 819 2 | 2HB | CYS A | 58154.570 | -8.947 | 0.835 | 1.00 | 0.00 H |
| ATOM | 820 | HG | CYS A | 58154.021 | -11.467 | -0.907 | 1.00 | 0.00 H |
| ATOM | 821 | N | ALAA | 59157.466 | 11.496 | 0.431 | 1.00 | 0.00 N |
| ATOM . | 822 | CA | ALA A | 59158.762 | -11.375 | -0.226 | 1.00 | 0.00 C |
| ATOM | 823 | C | ALA A | 59158.686 - | 10.433 | -1.423 | 1.00 | 0.00 C |
| ATOM | 824 | O | ALA A | 59157.969 | 10.698 | -2.389 | 1.00 | 0.00 O |
| ATOM | 825 | СВ | ALA A | 59159.262 | -12.744 | -0.661 | 1.00 | 0.00 C |
| ATOM | 826 | Н | ALA A | 59157.037 | 12.376 | 0.483 | 1.00 | 0.00 H |
| ATOM | 827 | НА | ALA A | 59159.463 | -10.974 | 0.491 | 1.00 | 0.00 H |
| ATOM | 828 | lНВ | ALA A | 59160.333 - | 12.710 | -0.800 | 1.00 | 0.00 H |
| ATOM | 829 2 | 2HB | ALA A | 59158.788 - | 13.021 | -1.592 | 1.00 | 0.00 H |
| ATOM | 830 3 | ВНВ | ALA A | 59159.020 - | 13.474 | 0.097 | 1.00 | 0.00 H |
| ATOM | 831 | N | GLY A | 60159.428 | -9.334 | -1.352 | 1.00 | 0.00 N |
| ATOM | 832 | CA | GLY A | 60159.430 | -8.369 | -2.437 | 1.00 | 0.00 C |
| ATOM | 833 | C | GLY A | 60158.687 | -7.096 | -2.082 | 1.00 | 0.00 C |
| ATOM | 834 | O | GLY A | 60157.935 | -6.561 | -2.896 | 1.00 | 0.00 O |
| ATOM | 835 | Н | GLY A | 60159.979 | -9.176 | -0.558 | 1.00 | 0.00 H |
| ATOM | 836 | lHA | GLY A | 60160.452 | -8.119 | -2.680 | 1.00 | 0.00 H |
| ATOM | 837 2 | 2HA | GLY A | 60158.963 | -8.816 | -3.302 | 1.00 | 0.00 H |
| ATOM | 838 | N | CYSA | 61158.897 | -6.610 | -0.863 | 1.00 | 0.00 N |
| ATOM | 839 | CA | CYS A | 61158.240 | -5.392 | -0.402 | 1.00 | 0.00 C |
| ATOM | 840 | C | CYS A | 61159.222 | -4.494 | 0.343 | 1.00 | 0.00 C |

| ATOM | 841 | Ο | CYS A | 61160.342 | -4.903 | 0.652 | 1.00 | 0.00 O |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 842 | CB | CYS A | 61157.058 | -5.738 | 0.505 | 1.00 | 0.00 C |
| ATOM | 843 | SG | CYSA | 61155.845 | -6.842 | -0.254 | 1.00 | 0.00 S |
| ATOM | 844 | Н | CYS A | 61159.508 | -7.081 | -0.258 | 1.00 | 0.00 H |
| ATOM | 845 | НА | CYS A | 61157.875 | -4.863 | -1.270 | 1.00 | 0.00 H |
| ATOM | 846 | 1HB | CYS A | 61157.427 | -6.219 | 1.397 | 1.00 | 0.00 H |
| ATOM | 847 | 2HB | CYS A | 61156.547 | -4.826 | 0.779 | 1.00 | 0.00 H |
| ATOM | 848 | HG | CYS A | 61154.969 | -6.511 | -0.042 | 1.00 | 0.00 H |
| ATOM | 849 | N | THR A | 62158.796 | -3.268 | 0.629 | 1.00 | 0.00 N |
| ATOM | 850 | CA | THR A | 62159.637 | -2.311 | 1.338 | 1.00 | 0.00 C |
| ATOM | 851 | C | THR A | 62159.197 | -2.171 | 2.790 | 1.00 | 0.00 C |
| ATOM | 852 | О | THR A | 62158.253 | -2.829 | 3.230 | 1.00 | 0.00 O |
| ATOM | 853 | CB | THR A | 62159.591 | -0.949 | 0.645 | 1.00 | 0.00 C |
| ATOM | 854 | OG1 | THR A | 62158.350 | -0.308 | 0.879 | 1.00 | 0.00 O |
| ATOM | 855 | CG2 | THR A | 62159.791 | -1.031 | -0.853 | 1.00 | 0.00 C |
| ATOM | 856 | Н | THR A | 62157.894 | -3.000 | 0.357 | 1.00 | 0.00 H |
| ATOM | 857 | НА | THR A | 62160.651 | -2.682 | 1.316 | 1.00 | 0.00 H |
| ATOM | 858 | НВ | THR A | 62160.376 | -0.325 | 1.050 | 1.00 | 0.00 H |
| ATOM | 859 | HG1 | THR A | 62157.639 | -0.850 | 0.529 | 1.00 | 0.00 H |
| ATOM | 860 | 1HG2 | THR A | 62158.928 | -1.498 | -1.305 | 1.00 | 0.00 H |
| ATOM | 861 | 2HG2 | THR A | 62160.671 | -1.618 | -1.067 | 1.00 | 0.00 H |
| ATOM | 862 | 3HG2 | THR A | 62159.913 | -0.036 | -1.254 | 1.00 | 0.00 H |
| ATOM | 863 | N | ASPA | 63159.886 | -1.310 | 3.533 | 1.00 | 0.00 N |
| ATOM | 864 | CA | ASPA | 63159.564 | -1.083 | 4.937 | 1.00 | 0.00 C |
| ATOM | 865 | C | ASPA | 63158.915 | 0.283 | 5.133 | 1.00 | 0.00 C |
| ATOM | 866 | О | ASPA | 63159.079 | 0.916 | 6.177 | 1.00 | 0.00 O |
| ATOM | 867 | CB | ASPA | 63160.827 | -1.189 | 5.794 | 1.00 | 0.00 C |

| ATOM | 868 | CG | ASPA | 63161.869 | -0.155 | 5.418 | 1.00 | 0.00 C | |
|------|-------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 869 | OD1 | ASP A | 63162.279 | 0.624 | 6.304 | 1.00 | 0.00 O | |
| ATOM | 870 | OD2 | ASP A | 63162.277 | -0.124 | 4.237 | 1.00 | 0.00 O | |
| ATOM | 871 | Н | ASPA | 63160.627 | -0.815 | 3.126 | 1.00 | 0.00 H | |
| ATOM | 872 | НА | ASPA | 63158.866 | -1.847 | 5.245 | 1.00 | 0.00 H | |
| ATOM | 873 1 | НВ | ASPA | 63160.564 | -1.046 | 6.832 | 1.00 | 0.00 H | |
| ATOM | 874 2 | HB | ASP A | 63161.258 | -2.171 | 5.668 | 1.00 | 0.00 H | |
| ATOM | 875 | N | GLY A | 64158.180 | 0.734 | 4.122 | 1.00 | 0.00 N | |
| ATOM | 876 | CA | GLY A | 64157.517 | 2.023 | 4.204 | 1.00 | 0.00 C | |
| ATOM | 877 | C | GLY A | 64158.203 | 3.081 | 3.362 | 1.00 | 0.00 C | |
| ATOM | 878 | O | GLY A | 64158.146 | 4.269 | 3.680 | 1.00 | 0.00 O | |
| ATOM | 879 | Н | GLY A | 64158.085 | 0.187 | 3.315 | 1.00 | 0.00 H | |
| ATOM | 880 1 | НА | GLY A | 64156.498 | 1.913 | 3.865 | 1.00 | 0.00 H | |
| ATOM | 881 2 | .HA | GLY A | 64157.511 | 2.347 | 5.233 | 1.00 | 0.00 H | |
| ATOM | 882 | N | THR A | 65158.852 | 2.650 | 2.285 | 1.00 | 0.00 N | |
| ATOM | 883 | CA | THR A | 65159.552 | 3.569 | 1.395 | 1.00 | 0.00 C | |
| ATOM | 884 | C | THR A | 65159.130 | 3.350 | -0.054 | 1.00 | 0.00 C | |
| ATOM | 885 | Ö | THR A | 65159.318 | 2.267 | -0.609 | 1.00 | 0.00 O | |
| ATOM | 886 | CB | THR A | 65161.065 | 3.392 | 1.530 | 1.00 | 0.00 C | |
| ATOM | 887 | OG1 | THR A | 65161.396 | 2.023 | 1.693 | 1.00 | 0.00 O | |
| ATOM | 888 | CG2 | THR A | 65161.654 | 4.148 | 2.700 | 1.00 | 0.00 C | |
| ATOM | 889 | Н | THR A | 65158.861 | 1.690 | 2.085 | 1.00 | 0.00 H | |
| ATOM | 890 | НА | THR A | 65159.290 | 4.576 | 1.685 | 1.00 | 0.00 H | |
| ATOM | 891 | НВ | THR A | 65161.541 | 3.751 | 0.629 | 1.00 | 0.00 H | |
| ATOM | 892 | HG1 | THR A | 65161.415 | 1.594 | 0.834 | 1.00 | 0.00 H | |
| ATOM | 893 1 | HG2 | THR A | 65160.857 | 4.539 | 3.315 | 1.00 | 0.00 H | |
| ATOM | 894 2 | HG2 | THR A | 65162.259 | 4.965 | 2.333 | 1.00 | 0.00 H | |

| ATOM | 895 | 3HG2 | THR A | 65162.268 | 3.482 | 3.288 | 1.00 | 0.00 H |
|--------|-----|------|-------|-----------|-------|--------|------|--------|
| ATOM | 896 | N | PHE A | 66158.560 | 4.385 | -0.663 | 1.00 | 0.00 N |
| ATOM | 897 | CA | PHE A | 66158.112 | 4.304 | -2.048 | 1.00 | 0.00 C |
| ATOM | 898 | C | PHE A | 66159.029 | 5.108 | -2.965 | 1.00 | 0.00 C |
| ATOM . | 899 | O | PHE A | 66159.115 | 6.331 | -2.857 | 1.00 | 0.00 O |
| ATOM | 900 | СВ | PHE A | 66156.675 | 4.814 | -2.172 | 1.00 | 0.00 C |
| ATOM | 901 | CG | PHE A | 66156.029 | 4.474 | -3.484 | 1.00 | 0.00 C |
| ATOM | 902 | CD1 | PHE A | 66155.625 | 5.475 | -4.354 | 1.00 | 0.00 C |
| ATOM | 903 | CD2 | PHE A | 66155.826 | 3.153 | -3.849 | 1.00 | 0.00 C |
| ATOM | 904 | CE1 | PHE A | 66155.032 | 5.165 | -5.562 | 1.00 | 0.00 C |
| ATOM | 905 | CE2 | PHE A | 66155.232 | 2.836 | -5.057 | 1.00 | 0.00 C |
| ATOM | 906 | CZ | PHE A | 66154.834 | 3.843 | -5.914 | 1.00 | 0.00 C |
| ATOM | 907 | Н | PHE A | 66158.438 | 5.222 | -0.168 | 1.00 | 0.00 H |
| ATOM | 908 | HA | PHE A | 66158.143 | 3.268 | -2.347 | 1.00 | 0.00 H |
| ATOM | 909 | 1HB | PHE A | 66156.077 | 4.380 | -1.385 | 1.00 | 0.00 H |
| ATOM | 910 | 2HB | PHE A | 66156.672 | 5.890 | -2.068 | 1.00 | 0.00 H |
| ATOM | 911 | HD1 | PHE A | 66155.780 | 6.509 | -4.080 | 1.00 | 0.00 H |
| ATOM | 912 | HD2 | PHE A | 66156.137 | 2.364 | -3.179 | 1.00 | 0.00 H |
| ATOM | 913 | HE1 | PHE A | 66154.721 | 5.954 | -6.231 | 1.00 | 0.00 H |
| ATOM | 914 | HE2 | PHE A | 66155.080 | 1.803 | -5.329 | 1.00 | H 00.0 |
| ATOM | 915 | HZ | PHE A | 66154.371 | 3.598 | -6.858 | 1.00 | 0.00 H |
| ATOM | 916 | N | ARG A | 67159.713 | 4.411 | -3.867 | 1.00 | 0.00 N |
| ATOM | 917 | CA | ARG A | 67160.624 | 5.059 | -4.803 | 1.00 | 0.00 C |
| ATOM | 918 | C | ARG A | 67161.735 | 5.794 | -4.062 | 1.00 | 0.00 C |
| ATOM | 919 | O | ARG A | 67162.174 | 6.864 | -4.482 | 1.00 | 0.00 O |
| ATOM | 920 | CB | ARG A | 67159.858 | 6.036 | -5.698 | 1.00 | 0.00 C |
| ATOM | 921 | CG | ARG A | 67158.819 | 5.365 | -6.581 | 1.00 | 0.00 C |

| ATOM | 922 | CD | ARG A | 67158.307 | 6.310 | -7.654 | 1.00 | 0.00 C |
|------|-------|------|-------|-----------|---------|---------|------|--------|
| ATOM | 923 | NE | ARG A | 67159.178 | 6.330 | -8.827 | 1.00 | 0.00 N |
| ATOM | 924 | CZ | ARG A | 67159.307 | 5.310 | -9.672 | 1.00 | 0.00 C |
| ATOM | 925 | NH1 | ARG A | 67158.624 | 4.189 | -9.480 | 1.00 | 0.00 N |
| ATOM | 926 | NH2 | ARG A | 67160.122 | 5.412 - | 10.714 | 1.00 | 0.00 N |
| ATOM | 927 | Н | ARG A | 67159.602 | 3.438 | -3.904 | 1.00 | 0.00 H |
| ATOM | 928 | НА | ARG A | 67161.066 | 4.291 | -5.420 | 1.00 | 0.00 H |
| ATOM | 929 | lНВ | ARG A | 67159.357 | 6.759 | -5.074 | 1.00 | 0.00 H |
| ATOM | 930 2 | 2HB | ARG A | 67160.564 | 6.549 | -6.336 | 1.00 | 0.00 H |
| ATOM | 931 | lHG | ARG A | 67159.266 | 4.504 | -7.056 | 1.00 | 0.00 H |
| ATOM | 932 2 | 2HG | ARG A | 67157.989 | 5.048 | -5.965 | 1.00 | 0.00 H |
| ATOM | 933 | IHD | ARG A | 67157.321 | 5.990 | -7.957 | 1.00 | 0.00 H |
| ATOM | 934 2 | 2HD | ARG A | 67158.250 | 7.306 | -7.242 | 1.00 | 0.00 H |
| ATOM | 935 | HE | ARG A | 67159.695 | 7.147 | -8.993 | 1.00 | 0.00 H |
| ATOM | 936 | 1HH1 | ARG A | 67158.008 | 4.106 | - 8.697 | 1.00 | 0.00 H |
| ATOM | 937 2 | 2HH1 | ARG A | 67158.725 | 3.426 - | 10.119 | 1.00 | 0.00 H |
| ATOM | 938 | 1HH2 | ARG A | 67160.639 | 6.254 - | 10.864 | 1.00 | 0.00 H |
| ATOM | 939 2 | 2HH2 | ARG A | 67160.219 | 4.646 - | 11.348 | 1.00 | 0.00 H |
| ATOM | 940 | N | GLY A | 68162.187 | 5.212 | -2.955 | 1.00 | 0.00 N |
| ATOM | 941 | CA | GLY A | 68163.243 | 5.827 | -2.173 | 1.00 | 0.00 C |
| ATOM | 942 | C | GLY A | 68162.762 | 7.037 | -1.396 | 1.00 | 0.00 C |
| ATOM | 943 | O | GLY A | 68163.536 | 7.953 | -1.119 | 1.00 | 0.00 O |
| ATOM | 944 | Н | GLY A | 68161.800 | 4.359 | -2.667 | 1.00 | 0.00 H |
| ATOM | 945 | 1HA | GLY A | 68163.632 | 5.098 | -1.478 | 1.00 | 0.00 H |
| ATOM | 946 | 2HA | GLY A | 68164.037 | 6.132 | -2.838 | 1.00 | 0.00 H |
| ATOM | 947 | N | THR A | 69161.481 | 7.040 | -1.044 | 1.00 | 0.00 N |
| ATOM | 948 | CA | THR A | 69160.897 | 8.147 | -0.295 | 1.00 | 0.00 C |

| ATOM | 949 | C | THR A | 69160.046 | 7.632 | 0.861 | 1.00 | 0.00 C |
|------|-------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 950 | О | THR A | 69158.867 | 7.323 | 0.687 | 1.00 | 0.00 O |
| ATOM | 951 | CB | THR A | 69160.049 | 9.023 | -1.217 | 1.00 | 0.00 C |
| ATOM | 952 | OG1 | THR A | 69160.737 | 9.293 | -2.425 | 1.00 | 0.00 O |
| ATOM | 953 | CG2 | THR A | 69159.669 | 10.351 | -0.598 | 1.00 | 0.00 C |
| ATOM | 954 | Н | THR A | 69160.914 | 6.280 | -1.294 | 1.00 | 0.00 H |
| ATOM | 955 | НА | THR A | 69161.706 | 8.738 | 0.105 | 1.00 | 0.00 H |
| ATOM | 956 | НВ | THR A | 69159.135 | 8.498 | -1.457 | 1.00 | 0.00 H |
| ATOM | 957 | HG1 | THR A | 69161.578 | 9.711 | -2.228 | 1.00 | 0.00 H |
| ATOM | 958 1 | HG2 | THR A | 69160.045 | 11.156 | -1.213 | 1.00 | 0.00 H |
| ATOM | 959 2 | HG2 | THR A | 69160.099 | 10.423 | 0.390 | 1.00 | 0.00 H |
| ATOM | 960 3 | HG2 | THR A | 69158.594 | 10.423 | -0.530 | 1.00 | 0.00 H |
| ATOM | 961 | N | ARG A | 70160.651 | 7.542 | 2.041 | 1.00 | 0.00 N |
| ATOM | 962 | CA | ARG A | 70159.949 | 7.064 | 3.226 | 1.00 | 0.00 C |
| ATOM | 963 | C | ARG A | 70158.808 | 8.005 | 3.600 | 1.00 | 0.00 C |
| ATOM | 964 | О | ARG A | 70158.979 | 9.224 | 3.623 | 1.00 | 0.00 O |
| ATOM | 965 | СВ | ARG A | 70160.920 | 6.931 | 4.401 | 1.00 | 0.00 C |
| ATOM | 966 | CG | ARG A | 70160.340 | 6.178 | 5.588 | 1.00 | 0.00 C |
| ATOM | 967 | CD | ARG A | 70160.741 | 6.817 | 6.909 | 1.00 | 0.00 C |
| ATOM | 968 | NE | ARG A | 70161.752 | 6.032 | 7.613 | 1.00 | 0.00 N |
| ATOM | 969 | CZ | ARG A | 70163.055 | 6.085 | 7.344 | 1.00 | 0.00 C |
| ATOM | 970 | NH1 | ARG A | 70163.511 | 6.883 | 6.385 | 1.00 | 0.00 N |
| ATOM | 971 | NH2 | ARG A | 70163.905 | 5.337 | 8.033 | 1.00 | 0.00 N |
| ATOM | 972 | Н | ARG A | 70161.592 | 7.802 | 2.115 | 1.00 | 0.00 H |
| ATOM | 973 | НА | ARG A | 70159.538 | 6.091 | 2.999 | 1.00 | 0.00 H |
| ATOM | 974 1 | НВ | ARG A | 70161.803 | 6.407 | 4.066 | 1.00 | 0.00 H |
| ATOM | 975 2 | HB | ARG A | 70161.203 | 7.920 | 4.732 | 1.00 | 0.00 H |

| ATOM | 976 | 1HG | ARG A | 70159.263 | 6.180 | 5.511 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 977 | 2HG | ARG A | 70160.703 | 5.159 | 5.566 | 1.00 | 0.00 H |
| ATOM | 978 | 1HD | ARG A | 70161.136 | 7.802 | 6.714 | 1.00 | 0.00 H |
| ATOM | 979 | 2HD | ARG A | 70159.863 | 6.899 | 7.533 | 1.00 | 0.00 H |
| ATOM | 980 | HE | ARG A | 70161.444 | 5.432 | 8.325 | 1.00 | 0.00 H |
| ATOM | 981 | 1HH1 | ARG A | 70162.877 | 7.450 | 5.861 | 1.00 | 0.00 H |
| ATOM | 982 | 2HH1 | ARG A | 70164.491 | 6.919 | 6.190 | 1.00 | 0.00 H |
| ATOM | 983 | 1HH2 | ARG A | 70163.567 | 4.734 | 8.756 | 1.00 | 0.00 H |
| ATOM | 984 | 2HH2 | ARG A | 70164.884 | 5.377 | 7.832 | 1.00 | 0.00 H |
| ATOM | 985 | N | TYR A | 71157.646 | 7.431 | 3.890 | 1.00 | 0.00 N |
| ATOM | 986 | CA | TYR A | 71156.476 | 8.218 | 4.264 | 1.00 | 0.00 C |
| ATOM | 987 | C | TYR A | 71156.055 | 7.920 | 5.700 | 1.00 | 0.00 C |
| ATOM | 988 | O | TYR A | 71155.648 | 8.817 | 6.437 | 1.00 | 0.00 O |
| ATOM | 989 | CB | TYRA | 71155.316 | 7.932 | 3.309 | 1.00 | 0.00 C |
| ATOM | 990 | CG | TYR A | 71155.479 | 8.569 | 1.948 | 1.00 | 0.00 C |
| ATOM | 991 | CD1 | TYR A | 71155.397 | 7.809 | 0.788 | 1.00 | 0.00 C |
| ATOM | 992 | CD2 | TYR A | 71155.717 | 9.933 | 1.823 | 1.00 | 0.00 C |
| ATOM | 993 | CE1 | TYR A | 71155.547 | 8.389 | -0.457 | 1.00 | 0.00 C |
| ATOM | 994 | CE2 | TYR A | 71155.867 | 10.520 | 0.581 | 1.00 | 0.00 C |
| ATOM | 995 | CZ | TYR A | 71155.781 | 9.745 | -0.555 | 1.00 | 0.00 C |
| ATOM | 996 | ОН | TYR A | 71155.931 | 10.325 | -1.793 | 1.00 | 0.00 O |
| ATOM | 997 | Н | TYR A | 71157.572 | 6.454 | 3.855 | 1.00 | 0.00 H |
| ATOM | 998 | HA | TYR A | 71156.742 | 9.262 | 4.190 | 1.00 | 0.00 H |
| ATOM | 999 | 1HB | TYR A | 71155.232 | 6.864 | 3.166 | 1.00 | 0.00 H |
| ATOM | 1000 | 2HB | TYR A | 71154.401 | 8.305 | 3.744 | 1.00 | 0.00 H |
| ATOM | 1001 | HD1 | TYR A | 71155.213 | 6.748 | 0.869 | 1.00 | 0.00 H |
| ATOM | 1002 | HD2 | TYRA | 71155.785 | 10.538 | 2.716 | 1.00 | 0.00 H |

| ATOM | 1003 | HE1 | TYR A | 71155.480 | 7.781 | -1.347 | 1.00 | 0.00 H |
|------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1004 | HE2 | TYR A | 71156.051 | 11.581 | 0.506 | 1.00 | 0.00 H |
| ATOM | 1005 | НН | TYR A | 71155.460 | 11.161 | -1.814 | 1.00 | 0.00 H |
| ATOM | 1006 | N | PHE A | 72156.155 | 6.653 | 6.089 | 1.00 | 0.00 N |
| ATOM | 1007 | CA | PHE A | 72155.784 | 6.235 | 7.436 | 1.00 | 0.00 C |
| ATOM | 1008 | C | PHE A | 72156.783 | 5.220 | 7.984 | 1.00 | 0.00 C |
| ATOM | 1009 | О | PHE A | 72157.758 | 4.872 | 7.320 | 1.00 | 0.00 O |
| ATOM | 1010 | СВ | PHE A | 72154.378 | 5.635 | 7.437 | 1.00 | 0.00 C |
| ATOM | 1011 | CG | PHE A | 72154.144 | 4.648 | 6.328 | 1.00 | 0.00 C |
| ATOM | 1012 | CD1 | PHE A | 72153.812 | 5.083 | 5.055 | 1.00 | 0.00 C |
| ATOM | 1013 | CD2 | PHE A | 72154.258 | 3.287 | 6.559 | 1.00 | 0.00 C |
| ATOM | 1014 | CE1 | PHE A | 72153.598 | 4.179 | 4.033 | 1.00 | 0.00 C |
| ATOM | 1015 | CE2 | PHE A | 72154.045 | 2.378 | 5.541 | 1.00 | 0.00 C |
| ATOM | 1016 | CZ | PHE A | 72153.714 | 2.824 | 4.276 | 1.00 | 0.00 C |
| ATOM | 1017 | Н | PHE A | 72156.486 | 5.982 | 5.455 | 1.00 | 0.00 H |
| ATOM | 1018 | HA | PHE A | 72155.795 | 7.110 | 8.068 | 1.00 | 0.00 H |
| ATOM | 1019 1 | HB | PHE A | 72154.212 | 5.125 | 8.375 | 1.00 | 0.00 H |
| ATOM | 1020 2 | 2HB | PHE A | 72153.654 | 6.431 | 7.333 | 1.00 | 0.00 H |
| ATOM | 1021 | HD1 | PHE A | 72153.721 | 6.142 | 4.864 | 1.00 | 0.00 H |
| ATOM | 1022 | HD2 | PHE A | 72154.517 | 2.937 | 7.548 | 1.00 | 0.00 H |
| ATOM | 1023 | HE1 | PHE A | 72153.338 | 4.530 | 3.045 | 1.00 | 0.00 H |
| ATOM | 1024 | HE2 | PHE A | 72154.137 | 1.319 | 5.734 | 1.00 | 0.00 H |
| ATOM | 1025 | HZ | PHE A | 72153.547 | 2.115 | 3.479 | 1.00 | 0.00 H |
| ATOM | 1026 | N | THR A | 73156.533 | 4.750 | 9.202 | 1.00 | 0.00 N |
| ATOM | 1027 | CA | THR A | 73157.409 | 3.775 | 9.840 | 1.00 | 0.00 C |
| ATOM | 1028 | C | THR A | 73156.665 | 2.470 | 10.108 | 1.00 | 0.00 C |
| ATOM | 1029 | О | THR A | 73155.816 | 2.398 | 10.997 | 1.00 | 0.00 O |

| ATOM | 1030 | CB | THR A | 73157.964 | 4.337 | 11.151 | 1.00 | 0.00 C |
|------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1031 | OG1 | THR A | 73157.040 | 5.231 | 11.743 | 1.00 | 0.00 O |
| ATOM | 1032 | CG2 | THR A | 73159.273 | 5.077 | 10.977 | 1.00 | 0.00 C |
| ATOM | 1033 | Н | THR A | 73155.738 | 5.066 | 9.682 | 1.00 | 0.00 H |
| ATOM | 1034 | HA | THR A | 73158.230 | 3.576 | 9.168 | 1.00 | 0.00 H |
| ATOM | 1035 | HB | THR A | 73158.133 | 3.520 | 11.837 | 1.00 | 0.00 H |
| ATOM | 1036 | HG1 | THR A | 73157.405 | 5.572 | 12.564 | 1.00 | 0.00 H |
| ATOM | 1037 | IHG2 | THR A | 73159.290 | 5.554 | 10.008 | 1.00 | 0.00 H |
| ATOM | 1038 2 | 2HG2 | THR A | 73160.093 | 4.377 | 11.048 | 1.00 | 0.00 H |
| ATOM | 1039 3 | 3HG2 | THR A | 73159.369 | 5.824 | 11.749 | 1.00 | 0.00 H |
| ATOM | 1040 | N | CYS A | 74156.991 | 1.440 | 9.335 | 1.00 | 0.00 N |
| ATOM | 1041 | CA | CYS A | 74156.354 | 0.138 | 9.488 | 1.00 | 0.00 C |
| ATOM | 1042 | C | CYS A | 74157.390 | -0.982 | 9.465 | 1.00 | 0.00 C |
| ATOM | 1043 | О | CYS A | 74158.591 | -0.728 | 9.368 | 1.00 | 0.00 O |
| ATOM | 1044 | CB | CYS A | 74155.323 | -0.083 | 8.379 | 1.00 | 0.00 C |
| ATOM | 1045 | SG | CYS A | 74153.706 | 0.652 | 8.718 | 1.00 | 0.00 S |
| ATOM | 1046 | Н | CYS A | 74157.676 | 1.559 | 8.643 | 1.00 | 0.00 H |
| ATOM | 1047 | HA | CYS A | 74155.850 | 0.125 | 10.442 | 1.00 | 0.00 H |
| ATOM | 1048 | lНВ | CYS A | 74155.694 | 0.350 | 7.462 | 1.00 | 0.00 H |
| ATOM | 1049 2 | 2HB | CYS A | 74155.180 | -1.144 | 8.237 | 1.00 | 0.00 H |
| ATOM | 1050 | HG | CYS A | 74153.749 | 1.078 | 9.577 | 1.00 | 0.00 H |
| ATOM | 1051 | N | ALA A | 75156.918 | -2.220 | 9.553 | 1.00 | 0.00 N |
| ATOM | 1052 | CA | ALA A | 75157.803 | -3.378 | 9.542 | 1.00 | 0.00 C |
| ATOM | 1053 | C | ALA A | 75158.397 | -3.602 | 8.156 | 1.00 | 0.00 C |
| ATOM | 1054 | О | ALA A | 75157.882 | -3.095 | 7.160 | 1.00 | 0.00 O |
| ATOM | 1055 | СВ | ALA A | 75157.053 | -4.619 | 10.004 | 1.00 | 0.00 C |
| ATOM | 1056 | Н | ALA A | 75155.951 | -2.359 | 9.628 | 1.00 | 0.00 H |

| ATOM | 1057 | HA | ALA A | 75158.605 | -3.190 | 10.241 | 1.00 | 0.00 H |
|------|------|----------|-------|-----------|---------|--------|------|--------|
| ATOM | 1058 | 1HB | ALA A | 75157.153 | -4.723 | 11.074 | 1.00 | 0.00 H |
| ATOM | 1059 | 2HB | ALA A | 75157.466 | -5.490 | 9.518 | 1.00 | 0.00 H |
| ATOM | 1060 | 3НВ | ALA A | 75156.008 | -4.525 | 9.747 | 1.00 | 0.00 H |
| ATOM | 1061 | N | LEU A | 76159.484 | -4.366 | 8.100 | 1.00 | 0.00 N |
| ATOM | 1062 | CA | LEU A | 76160.148 | -4.658 | 6.836 | 1.00 | 0.00 C |
| ATOM | 1063 | C | LEU A | 76159.378 | -5.712 | 6.046 | 1.00 | 0.00 C |
| ATOM | 1064 | О | LEU A | 76158.795 | -6.631 | 6.623 | 1.00 | 0.00 O |
| ATOM | 1065 | CB | LEU A | 76161.579 | -5.137 | 7.087 | 1.00 | 0.00 C |
| ATOM | 1066 | CG | LEU A | 76162.627 | -4.025 | 7.176 | 1.00 | 0.00 C |
| ATOM | 1067 | CD1 | LEU A | 76163.728 | -4.406 | 8.153 | 1.00 | 0.00 C |
| ATOM | 1068 | CD2 | LEUA | 76163.208 | - 3.731 | 5.802 | 1.00 | 0.00 C |
| ATOM | 1069 | H | LEU A | 76159.846 | -4.742 | 8.929 | 1.00 | 0.00 H |
| ATOM | 1070 | HA | LEU A | 76160.179 | -3.745 | 6.259 | 1.00 | 0.00 H |
| ATOM | 1071 | 1HB | LEU A | 76161.593 | -5.692 | 8.013 | 1.00 | 0.00 H |
| ATOM | 1072 | 2HB | LEU A | 76161.861 | -5.800 | 6.284 | 1.00 | 0.00 H |
| ATOM | 1073 | HG | LEU A | 76162.155 | -3.124 | 7.541 | 1.00 | 0.00 H |
| ATOM | 1074 | 1HD1 | LEU A | 76164.661 | -3.965 | 7.834 | 1.00 | 0.00 H |
| ATOM | 1075 | 2HD1 | LEU A | 76163.828 | -5.481 | 8.180 | 1.00 | 0.00 H |
| ATOM | 1076 | 3HD1 | LEU A | 76163.476 | -4.044 | 9.139 | 1.00 | 0.00 H |
| ATOM | 1077 | 1HD2 | LEU A | 76164.135 | -4.272 | 5.681 | 1.00 | 0.00 H |
| ATOM | 1078 | 2HD2 | LEU A | 76163.395 | -2.671 | 5.708 | 1.00 | 0.00 H |
| ATOM | 1079 | 3HD2 | LEU A | 76162.508 | -4.041 | 5.040 | 1.00 | 0.00 H |
| ATOM | 1080 | N | LYS A | 77159.379 | -5.572 | 4.724 | 1.00 | 0.00 N |
| ATOM | 1081 | CA | LYS A | 77158.681 | -6.513 | 3.857 | 1.00 | 0.00 C |
| ATOM | 1082 | C | LYS A | 77157.188 | -6.536 | 4.170 | 1.00 | 0.00 C |
| ATOM | 1083 | O | LYS A | 77156.545 | -7.584 | 4.103 | 1.00 | 0.00 O |

| ATOM | 1084 | CB | LYS A | 77159.268 | -7.917 | 4.011 | 1.00 | 0.00 C |
|------|---------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1085 | CG | LYS A | 77160.742 | -8.002 | 3.648 | 1.00 | 0.00 C |
| ATOM | 1086 | CD | LYS A | 77160.936 | -8.190 | 2.152 | 1.00 | 0.00 C |
| ATOM | 1087 | CE | LYS A | 77162.179 | -7.470 | 1.656 | 1.00 | 0.00 C |
| ATOM | 1088 | NZ | LYS A | 77162.702 | -8.067 | 0.396 | 1.00 | 0.00 N |
| ATOM | 1089 | Н | LYS A | 77159.861 | -4.819 | 4.324 | 1.00 | 0.00 H |
| ATOM | 1090 | НА | LYS A | 77158.816 | -6.185 | 2.837 | 1.00 | 0.00 H |
| ATOM | 1091 1 | НВ | LYS A | 77159.154 | -8.231 | 5.038 | 1.00 | 0.00 H |
| ATOM | .1092 2 | 2HB | LYS A | 77158.722 | -8.595 | 3.373 | 1.00 | 0.00 H |
| ATOM | 1093 1 | HG | LYS A | 77161.232 | -7.089 | 3.952 | 1.00 | 0.00 H |
| ATOM | 1094 2 | 2HG | LYS A | 77161.183 | -8.840 | 4.168 | 1.00 | 0.00 H |
| ATOM | 1095 1 | HD | LYS A | 77161.036 | -9.245 | 1.942 | 1.00 | 0.00 H |
| ATOM | 1096 2 | 2HD | LYS A | 77160.073 | -7.799 | 1.634 | 1.00 | 0.00 H |
| ATOM | 1097 1 | HE | LYS A | 77161.932 | -6.434 | 1.478 | 1.00 | 0.00 H |
| ATOM | 1098 2 | 2HE | LYS A | 77162.943 | -7.531 | 2.418 | 1.00 | 0.00 H |
| ATOM | 1099 1 | HZ | LYS A | 77162.608 | -9.102 | 0.425 | 1.00 | 0.00 H |
| ATOM | 1100 2 | HZ | LYS A | 77163.706 | -7.824 | 0.274 | 1.00 | 0.00 H |
| ATOM | 1101 3 | BHZ | LYS A | 77162.168 | -7.703 | -0.419 | 1.00 | 0.00 H |
| ATOM | 1102 | N | LYS A | 78156.643 | -5.373 | 4.513 | 1.00 | 0.00 N |
| ATOM | 1103 | CA | LYS A | 78155.224 | -5.259 | 4.837 | 1.00 | 0.00 C |
| ATOM | 1104 | C | LYS A | 78154.686 | -3.886 | 4.449 | 1.00 | 0.00 C |
| ATOM | 1105 | О | LYS A | 78153.863 | -3.308 | 5.158 | 1.00 | 0.00 O |
| ATOM | 1106 | CB | LYS A | 78155.000 | -5.505 | 6.330 | 1.00 | 0.00 C |
| ATOM | 1107 | CG | LYS A | 78155.513 | -6.854 | 6.809 | 1.00 | 0.00 C |
| ATOM | 1108 | CD | LYS A | 78155.303 | -7.030 | 8.304 | 1.00 | 0.00 C |
| ATOM | 1109 | CE | LYSA | 78154.065 | -7.862 | 8.598 | 1.00 | 0.00 C |
| ATOM | 1110 | ΝZ | LYS A | 78153.334 | -7.367 | 9.797 | 1.00 | 0.00 N |

| ATOM | 1111 F | H LYS A | 78157.206 | -4.572 | 4.548 | 1.00 | 0.00 H |
|------|---------|----------|-----------|--------|--------|------|--------|
| ATOM | 1112 I | HA LYSA | 78154.695 | -6.012 | 4.274 | 1.00 | 0.00 H |
| ATOM | 1113 1H | IB LYS A | 78155.507 | -4.732 | 6.890 | 1.00 | 0.00 H |
| ATOM | 1114 2H | IB LYS A | 78153.942 | -5.453 | 6.537 | 1.00 | 0.00 H |
| ATOM | 1115 1H | IG LYS A | 78154.984 | -7.636 | 6.285 | 1.00 | 0.00 H |
| ATOM | 1116 2H | IG LYS A | 78156.570 | -6.924 | 6.592 | 1.00 | 0.00 H |
| ATOM | 1117 1H | ID LYS A | 78156.165 | -7.526 | 8.723 | 1.00 | 0.00 H |
| ATOM | 1118 2H | ID LYS A | 78155.188 | -6.057 | 8.759 | 1.00 | 0.00 H |
| ATOM | 1119 1H | IE LYSA | 78153.407 | -7.820 | 7.743 | 1.00 | 0.00 H |
| ATOM | 1120 2H | HE LYSA | 78154.367 | -8.886 | 8.768 | 1.00 | 0.00 H |
| ATOM | 1121 1H | HZ LYS A | 78152.990 | -6.399 | 9.630 | 1.00 | 0.00 H |
| ATOM | 1122 2H | IZ LYS A | 78153.965 | -7.361 | 10.623 | 1.00 | 0.00 H |
| ATOM | 1123 3H | IZ LYS A | 78152.521 | -7.982 | 9.999 | 1.00 | 0.00 H |
| ATOM | 1124 | N ALAA | 79155.156 | -3.369 | 3.318 | 1.00 | 0.00 N |
| ATOM | 1125 | CA ALAA | 79154.722 | -2.064 | 2.836 | 1.00 | 0.00 C |
| ATOM | 1126 | C ALAA | 79154.543 | -2.070 | 1.322 | 1.00 | 0.00 C |
| ATOM | 1127 | O ALAA | 79155.517 | -1.992 | 0.571 | 1.00 | 0.00 O |
| ATOM | 1128 | CB ALAA | 79155.720 | -0.992 | 3.247 | 1.00 | 0.00 C |
| ATOM | 1129 I | H ALAA | 79155.811 | -3.879 | 2.796 | 1.00 | 0.00 H |
| ATOM | 1130 I | HA ALAA | 79153.774 | -1.837 | 3.299 | 1.00 | 0.00 H |
| ATOM | 1131 1E | IB ALAA | 79155.219 | -0.036 | 3.300 | 1.00 | 0.00 H |
| ATOM | 1132 2H | IB ALAA | 79156.515 | -0.941 | 2.518 | 1.00 | 0.00 H |
| ATOM | 1133 3H | IB ALAA | 79156.133 | -1.237 | 4.214 | 1.00 | 0.00 H |
| ATOM | 1134 | N LEUA | 80153.294 | -2.162 | 0.878 | 1.00 | 0.00 N |
| ATOM | 1135 | CA LEUA | 80152.988 | -2.178 | -0.548 | 1.00 | 0.00 C |
| ATOM | 1136 | C LEUA | 80152.143 | -0.968 | -0.936 | 1.00 | 0.00 C |
| ATOM | 1137 | O LEUA | 80150.992 | -0.842 | -0.519 | 1.00 | 0.00 O |

| ATOM | 1138 | CB | LEU A | 80152.252 | -3.467 | -0.919 | 1.00 | 0.00 C |
|--------|--------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1139 | CG | LEU A | 80151.835 | -3.574 | -2.387 | 1.00 | 0.00 C |
| ATOM | 1140 | CD1 | LEU A | 80153.048 | -3.819 | -3.270 | 1.00 | 0.00 C |
| ATOM | 1141 | CD2 | LEU A | 80150.809 | -4.683 | -2.568 | 1.00 | 0.00 C |
| ATOM | 1142 | Н | LEU A | 80152.561 | -2.220 | 1.525 | 1.00 | 0.00 H |
| ATOM | 1143 | НА | LEU A | 80153.922 | -2.138 | -1.088 | 1.00 | 0.00 H |
| ATOM | 1144 | lНВ | LEU A | 80152.896 | -4.303 | -0.687 | 1.00 | 0.00 H |
| ATOM | 1145 2 | 2HB | LEU A | 80151.364 | -3.538 | -0.309 | 1.00 | 0.00 H |
| ATOM | 1146 | HG | LEU A | 80151.381 | -2.644 | -2.693 | 1.00 | 0.00 H |
| ATOM | 1147 | HD1 | LEU A | 80153.457 | -2.872 | -3.590 | 1.00 | 0.00 H |
| ATOM | 1148 2 | 2HD1 | LEU A | 80152.753 | -4.394 | -4.136 | 1.00 | 0.00 H |
| ATOM | 11493 | 3HD1 | LEU A | 80153.796 | -4.364 | -2.713 | 1.00 | 0.00 H |
| ATOM | 1150 | HD2 | LEU A | 80150.935 | -5.134 | -3.541 | 1.00 | 0.00 H |
| ATOM | 11512 | 2HD2 | LEU A | 80149.814 | -4.270 | -2.488 | 1.00 | 0.00 H |
| ATOM | 1152 | 3HD2 | LEU A | 80150.950 | -5.432 | -1.803 | 1.00 | 0.00 H |
| ATOM | 1153 | N | PHE A | 81152.723 | -0.082 | -1.739 | 1.00 | 0.00 N |
| ATOM | 1154 | CA | PHE A | 81152.024 | 1.117 | -2.185 | 1.00 | 0.00 C |
| ATOM | 1155 | C | PHE A | 81151.158 | 0.819 | -3.405 | 1.00 | 0.00 C |
| ATOM | 1156 | O | PHE A | 81151.569 | 0.089 | -4.307 | 1.00 | 0.00 O |
| ATOM | 1157 | CB | PHE A | 81153.027 | 2.224 | -2.515 | 1.00 | 0.00 C |
| ATOM | 1158 | CG | PHE A | 81153.688 | 2.816 | -1.303 | 1.00 | 0.00 C |
| ATOM | 1159 | CD1 | PHE A | 81153.308 | 4.060 | -0.828 | 1.00 | 0.00 C |
| ATOM | 1160 | CD2 | PHE A | 81154.690 | 2.126 | -0.639 | 1.00 | 0.00 C |
| ATOM | 1161 | CE1 | PHE A | 81153.915 | 4.607 | 0.287 | 1.00 | 0.00 C |
| ATOM | 1162 | CE2 | PHE A | 81155.300 | 2.668 | 0.477 | 1.00 | 0.00 C |
| ATOM . | 1163 | CZ | PHE A | 81154.912 | 3.909 | 0.941 | 1.00 | 0.00 C |
| ATOM | 1164 | Н | PHE A | 81153.643 | -0.239 | -2.039 | 1.00 | 0.00 H |

| ATOM | 1165 | HA | PHE A | 81151.388 | 1.449 | -1.379 | 1.00 | 0.00 H | |
|------|--------|-----|-------|-----------|--------|--------|------|--------|--|
| ATOM | 1166 1 | НВ | PHE A | 81153.800 | 1.822 | -3.151 | 1.00 | 0.00 H | |
| ATOM | 1167 2 | НВ | PHE A | 81152.515 | 3.020 | -3.037 | 1.00 | 0.00 H | |
| ATOM | 1168 | HD1 | PHE A | 81152.527 | 4.606 | -1.338 | 1.00 | 0.00 H | |
| ATOM | 1169 | HD2 | PHE A | 81154.995 | 1.156 | -1.000 | 1.00 | 0.00 H | |
| ATOM | 1170 | HE1 | PHE A | 81153.609 | 5.579 | 0.647 | 1.00 | 0.00 H | |
| ATOM | 1171 | HE2 | PHE A | 81156.080 | 2.121 | 0.985 | 1.00 | 0.00 H | |
| ATOM | 1172 | HZ | PHE A | 81155.388 | 4.335 | 1.812 | 1.00 | 0.00 H | |
| ATOM | 1173 | N | VAL A | 82149.959 | 1.389 | -3.427 | 1.00 | 0.00 N | |
| ATOM | 1174 | CA | VAL A | 82149.035 | 1.184 | -4.535 | 1.00 | 0.00 C | |
| ATOM | 1175 | C | VALA | 82148.156 | 2.412 | -4.753 | 1.00 | 0.00 C | |
| ATOM | 1176 | O | VAL A | 82148.101 | 3.306 | -3.909 | 1.00 | 0.00 O | |
| ATOM | 1177 | CB | VALA | 82148.134 | -0.041 | -4.297 | 1.00 | 0.00 C | |
| ATOM | 1178 | CG1 | VAL A | 82148.953 | -1.322 | -4.333 | 1.00 | 0.00 C | |
| ATOM | 1179 | CG2 | VAL A | 82147.392 | 0.090 | -2.976 | 1.00 | 0.00 C | |
| ATOM | 1180 | Н | VAL A | 82149.687 | 1.962 | -2.677 | 1.00 | 0.00 H | |
| ATOM | 1181 | НА | VAL A | 82149.619 | 1.009 | -5.427 | 1.00 | 0.00 H | |
| ATOM | 1182 | HB | VAL A | 82147.404 | -0.087 | -5.093 | 1.00 | 0.00 H | |
| ATOM | 1183 1 | HG1 | VAL A | 82148.303 | -2.170 | -4.174 | 1.00 | 0.00 H | |
| ATOM | 1184 2 | HG1 | VAL A | 82149.702 | -1.292 | -3.555 | 1.00 | 0.00 H | |
| ATOM | 1185 3 | HG1 | VAL A | 82149.436 | -1.415 | -5.295 | 1.00 | 0.00 H | |
| ATOM | 1186 1 | HG2 | VAL A | 82147.988 | -0.338 | -2.185 | 1.00 | 0.00 H | |
| ATOM | 1187 2 | HG2 | VAL A | 82146.449 | -0.432 | -3.039 | 1.00 | 0.00 H | |
| ATOM | 1188 3 | HG2 | VAL A | 82147.212 | 1.134 | -2.767 | 1.00 | 0.00 H | |
| ATOM | 1189 | N | LYS A | 83147.471 | 2.448 | -5.891 | 1.00 | 0.00 N | |
| ATOM | 1190 | CA | LYS A | 83146.594 | 3.565 | -6.221 | 1.00 | 0.00 C | |
| ATOM | 1191 | C | LYS A | 83145.381 | 3.596 | -5.299 | 1.00 | 0.00 C | |

| ATOM | 1192 O | LYS A | 83144.624 | 2.629 | -5.217 | 1.00 | 0.00 O |
|------|----------|----------|-----------|----------|--------|------|--------|
| ATOM | 1193 CB | LYS A | 83146.139 | 3.470 | -7.679 | 1.00 | 0.00 C |
| ATOM | 1194 CG | LYS A | 83147.278 | 3.584 | -8.680 | 1.00 | 0.00 C |
| ATOM | 1195 CD | LYSA | 83146.839 | 3.163 - | 10.073 | 1.00 | 0.00 C |
| ATOM | 1196 CE | LYS A | 83147.457 | 4.048 - | 11.143 | 1.00 | 0.00 C |
| ATOM | 1197 NZ | LYSA | 83147.818 | 3.274 - | 12.363 | 1.00 | 0.00 N |
| ATOM | 1198 H | LYS A | 83147.557 | 1.704 | -6.524 | 1.00 | 0.00 H |
| ATOM | 1199 HA | LYS A | 83147.155 | 4.478 | -6.087 | 1.00 | 0.00 H |
| ATOM | 1200 1HB | LYS A | 83145.649 | 2.520 | -7.830 | 1.00 | 0.00 H |
| ATOM | 1201 2HB | LYS A | 83145.434 | 4.265 | -7.876 | 1.00 | 0.00 H |
| ATOM | 1202 1HG | LYS A | 83147.612 | 4.610 | -8.714 | 1.00 | 0.00 H |
| ATOM | 1203 2HG | LYS A | 83148.090 | 2.948 | -8.359 | 1.00 | 0.00 H |
| ATOM | 1204 1HD | LYS A | 83147.145 | 2.142 - | 10.243 | 1.00 | 0.00 H |
| ATOM | 1205 2HD | LYS A | 83145.763 | 3.233 - | 10.137 | 1.00 | 0.00 H |
| ATOM | 1206 1HE | LYS A | 83146.748 | 4.815 -1 | 1.411 | 1.00 | 0.00 H |
| ATOM | 1207 2HE | LYS A | 83148.348 | 4.506 -1 | 0.741 | 1.00 | 0.00 H |
| ATOM | 1208 1HZ | LYS A | 83148.624 | 3.721 -1 | 12.844 | 1.00 | 0.00 H |
| ATOM | 1209 2HZ | LYS A | 83147.011 | 3.243 -1 | 3.018 | 1.00 | 0.00 H |
| ATOM | 1210 3HZ | LYS A | 83148.078 | 2.300 -1 | 12.105 | 1.00 | 0.00 H |
| ATOM | 1211 N | LEU A | 84145.203 | 4.715 | -4.606 | 1.00 | 0.00 N |
| ATOM | 1212 CA | LEU A | 84144.082 | 4.880 | -3.689 | 1.00 | 0.00 C |
| ATOM | 1213 C | LEU A | 84142.752 | 4.717 | -4.418 | 1.00 | 0.00 C |
| ATOM | 1214 O | LEU A | 84141.808 | 4.136 | -3.885 | 1.00 | 0.00 O |
| ATOM | 1215 CE | B LEU A | 84144.149 | 6.254 | -3.018 | 1.00 | 0.00 C |
| ATOM | 1216 CC | G LEUA | 84142.966 | 6.592 | -2.109 | 1.00 | 0.00 C |
| ATOM | 1217 CI | O1 LEU A | 84143.161 | 5.981 | -0.730 | 1.00 | 0.00 C |
| ATOM | 1218 CI | 2 LEU A | 84142.791 | 8.100 | -2.004 | 1.00 | 0.00 C |

| ATOM | 1219 | Н | LEU A | 84145.841 | 5.450 | -4.716 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|---------|--------|------|--------|
| ATOM | 1220 | HA | LEU A | 84144.160 | 4.115 | -2.931 | 1.00 | 0.00 H |
| ATOM | 1221 | 1HB | LEU A | 84145.054 | 6.300 | -2.429 | 1.00 | 0.00 H |
| ATOM | 1222 | 2HB | LEU A | 84144.206 | 7.004 | -3.793 | 1.00 | 0.00 H |
| ATOM | 1223 | HG | LEU A | 84142.063 | 6.179 | -2.533 | 1.00 | 0.00 H |
| ATOM | 1224 | 1HD1 | LEU A | 84142.445 | 6.406 | -0.043 | 1.00 | 0.00 H |
| ATOM | 1225 | 2HD1 | LEU A | 84144.162 | 6.188 | -0.382 | 1.00 | 0.00 H |
| ATOM | 1226 | 3HD1 | LEU A | 84143.014 | 4.912 | -0.787 | 1.00 | 0.00 H |
| ATOM | 1227 | 1HD2 | LEU A | 84142.772 | 8.530 | -2.995 | 1.00 | 0.00 H |
| ATOM | 1228 | 2HD2 | LEU A | 84143.614 | 8.521 | -1.445 | 1.00 | 0.00 H |
| ATOM | 1229 | 3HD2 | LEU A | 84141.863 | 8.321 | -1.498 | 1.00 | 0.00 H |
| ATOM | 1230 | N | LYS A | 85142.688 | 5.234 | -5.641 | 1.00 | 0.00 N |
| ATOM | 1231 | CA | LYS A | 85141.474 | 5.146 | -6.444 | 1.00 | 0.00 C |
| ATOM | 1232 | C | LYS A | 85141.139 | 3.693 | -6.773 | 1.00 | 0.00 C |
| ATOM | 1233 | О | LYS A | 85139.984 | 3.356 | -7.028 | 1.00 | 0.00 O |
| ATOM | 1234 | СВ | LYS A | 85141.633 | 5.950 | -7.735 | 1.00 | 0.00 C |
| ATOM | 1235 | CG | LYS A | 85142.797 | 5.492 | -8.599 | 1.00 | 0.00 C |
| ATOM | 1236 | CD | LYSA | 85143.178 | 6.548 | -9.624 | 1.00 | 0.00 C |
| ATOM | 1237 | CE | LYS A | 85144.685 | 6.620 | -9.814 | 1.00 | 0.00 C |
| ATOM | 1238 | NZ | LYS A | 85145.077 | 7.728 - | 10.729 | 1.00 | 0.00 N |
| ATOM | 1239 | Н | LYS A | 85143.474 | 5.685 | -6.012 | 1.00 | 0.00 H |
| ATOM | 1240 | НА | LYSA | 85140.664 | 5.566 | -5.867 | 1.00 | 0.00 H |
| ATOM | 1241 | 1HB | LYS A | 85140.726 | 5.860 | -8.316 | 1.00 | 0.00 H |
| ATOM | 1242 | 2HB | LYS A | 85141.786 | 6.989 | -7.483 | 1.00 | 0.00 H |
| ATOM | 1243 | 1HG | LYS A | 85143.648 | 5.297 | -7.964 | 1.00 | 0.00 H |
| ATOM | 1244 | 2HG | LYS A | 85142.515 | 4.586 | -9.115 | 1.00 | 0.00 H |
| ATOM | 1245 | 1HD | LYS A | 85142.718 | 6.301 - | 10.569 | 1.00 | 0.00 H |

| ATOM | 1246 2HD | LYS A | 85142.820 | 7.509 | -9.287 | 1.00 | 0.00 H |
|--------|----------|---------|-----------|---------|--------|------|--------|
| ATOM | 1247 1HE | LYS A | 85145.149 | 6.779 | -8.852 | 1.00 | 0.00 H |
| ATOM | 1248 2HE | LYS A | 85145.028 | 5.683 - | 10.228 | 1.00 | 0.00 H |
| ATOM | 1249 1HZ | LYS A | 85146.064 | 8.004 - | 10.553 | 1.00 | 0.00 H |
| ATOM | 1250 2HZ | LYS A | 85144.465 | 8.553 - | 10.574 | 1.00 | 0.00 H |
| ATOM | 1251 3HZ | LYS A | 85144.984 | 7.423 - | 11.719 | 1.00 | 0.00 H |
| ATOM | 1252 N | SER A | 86142.158 | 2.837 | -6.765 | 1.00 | 0.00 N |
| ATOM | 1253 CA | SER A | 86141.968 | 1.423 | -7.064 | 1.00 | 0.00 C |
| ATOM | 1254 C | SER A | 86141.945 | 0.594 | -5.782 | 1.00 | 0.00 C |
| ATOM | 1255 O | SER A | 86142.403 | -0.548 | -5.762 | 1.00 | 0.00 O |
| ATOM | 1256 CB | SER A | 86143.077 | 0.922 | -7.990 | 1.00 | 0.00 C |
| ATOM | 1257 OC | SER A | 86143.061 | 1.613 | -9.227 | 1.00 | 0.00 O |
| ATOM | 1258 H | SER A | 86143.057 | 3.164 | -6.555 | 1.00 | 0.00 H |
| ATOM | 1259 HA | SER A | 86141.017 | 1.314 | -7.563 | 1.00 | 0.00 H |
| ATOM | 1260 1HB | SER A | 86144.035 | 1.078 | -7.518 | 1.00 | 0.00 H |
| ATOM | 1261 2HB | · SER A | 86142.936 | -0.133 | -8.178 | 1.00 | 0.00 H |
| ATOM · | 1262 HC | SER A | 86142.156 | 1.684 | -9.542 | 1.00 | 0.00 H |
| ATOM | 1263 N | CYS A | 87141.410 | 1.178 | -4.715 | 1.00 | 0.00 N |
| ATOM | 1264 CA | CYSA | 87141.328 | 0.494 | -3.430 | 1.00 | 0.00 C |
| ATOM | 1265 C | CYS A | 87139.877 | 0.215 | -3.053 | 1.00 | 0.00 C |
| ATOM | 1266 O | CYSA | 87138.984 | 1.005 | -3.360 | 1.00 | 0.00 O |
| ATOM | 1267 CE | CYS A | 87141.999 | 1.331 | -2.340 | 1.00 | 0.00 C |
| ATOM | 1268 SC | CYSA | 87143.804 | 1.366 | -2.440 | 1.00 | 0.00 S |
| ATOM | 1269 H | CYS A | 87141.062 | 2.090 | -4.794 | 1.00 | 0.00 H |
| ATOM | 1270 HA | A CYS A | 87141.851 | -0.446 | -3.521 | 1.00 | 0.00 H |
| ATOM | 1271 1HB | CYS A | 87141.648 | 2.350 | -2.411 | 1.00 | 0.00 H |
| ATOM | 1272 2HB | CYS A | 87141.730 | 0.931 | -1.372 | 1.00 | 0.00 H |

| ATOM | 1273 | HG | CYS A | 87144.150 | 1.419 | -1.547 | 1.00 | 0.00 H |
|------|------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 1274 | N | ARG A | 88139.650 | -0.912 | -2.386 | 1.00 | 0.00 N |
| ATOM | 1275 | CA | ARG A | 88138.306 | -1.294 | -1.967 | 1.00 | 0.00 C |
| ATOM | 1276 | C | ARG A | 88138.213 | -1.371 | -0.443 | 1.00 | 0.00 C |
| ATOM | 1277 | О | ARG A | 88139.151 | -1.815 | 0.220 | 1.00 | 0.00 O |
| ATOM | 1278 | CB | ARG A | 88137.922 | -2.641 | -2.582 | 1.00 | 0.00 C |
| ATOM | 1279 | CG | ARG A | 88137.196 | -2.517 | -3.912 | 1.00 | 0.00 C |
| ATOM | 1280 | CD | ARG A | 88135.691 | -2.650 | -3.741 | 1.00 | 0.00 C |
| ATOM | 1281 | NE | ARG A | 88135.014 | -2.887 | -5.014 | 1.00 | 0.00 N |
| ATOM | 1282 | CZ | ARG A | 88135.048 | -4.047 | -5.667 | 1.00 | 0.00 C |
| ATOM | 1283 | NH1 | ARG A | 88135.722 | -5.076 | -5.171 | 1.00 | 0.00 N |
| ATOM | 1284 | NH2 | ARG A | 88134.404 | -4.178 | -6.818 | 1.00 | 0.00 N |
| ATOM | 1285 | Н | ARG A | 88140.403 | -1.499 | -2.170 | 1.00 | 0.00 H |
| ATOM | 1286 | HA | ARG A | 88137.622 | -0.538 | -2.321 | 1.00 | 0.00 H |
| ATOM | 1287 | 1HB | ARG A | 88138.819 | -3.221 | -2.738 | 1.00 | 0.00 H |
| ATOM | 1288 | 2HB | ARG A | 88137.278 | -3.168 | -1.893 | 1.00 | 0.00 H |
| ATOM | 1289 | 1HG | ARG A | 88137.415 | -1.551 | -4.342 | 1.00 | 0.00 H |
| ATOM | 1290 | 2HG | ARG A | 88137.545 | -3.296 | -4.575 | 1.00 | 0.00 H |
| ATOM | 1291 | 1HD | ARG A | 88135.489 | -3.478 | -3.078 | 1.00 | 0.00 H |
| ATOM | 1292 | 2HD | ARG A | 88135.310 | -1.739 | -3.305 | 1.00 | 0.00 H |
| ATOM | 1293 | HE | ARG A | 88134.509 | -2.143 | -5.402 | 1.00 | 0.00 H |
| ATOM | 1294 | 1HH1 | ARG A | 88136.210 | -4.985 | -4.303 | 1.00 | 0.00 H |
| ATOM | 1295 | 2HH1 | ARG A | 88135.743 | -5.945 | -5.665 | 1.00 | 0.00 H |
| ATOM | 1296 | 1HH2 | ARG A | 88133.894 | -3.405 | -7.196 | 1.00 | 0.00 H |
| ATOM | 1297 | 2HH2 | ARG A | 88134.428 | -5.048 | -7.309 | 1.00 | 0.00 H |
| ATOM | 1298 | N | PRO A | 89137.078 | -0.939 | 0.135 | 1.00 | 0.00 N |
| ATOM | 1299 | CA | PRO A | 89136.874 | -0.966 | 1.588 | 1.00 | 0.00 C |

| ATOM | 1300 | C | PRO A | 89137.102 | -2.352 | 2.179 | 1.00 | 0.00 C |
|------|--------|-----|-------|-----------|---------|--------|------|--------|
| ATOM | 1301 | О | PRO A | 89136.511 | -3.334 | 1.728 | 1.00 | 0.00 O |
| ATOM | 1302 | CB | PRO A | 89135.410 | -0.549 | 1.755 | 1.00 | 0.00 C |
| ATOM | 1303 | CG | PRO A | 89135.090 | 0.225 | 0.523 | 1.00 | 0.00 C |
| ATOM | 1304 | CD | PRO A | 89135.907 | -0.394 | -0.577 | 1.00 | 0.00 C |
| ATOM | 1305 | HA | PRO A | 89137.513 | -0.254 | 2.089 | 1.00 | 0.00 H |
| ATOM | 1306 | lНВ | PRO A | 89134.791 | -1.430 | 1.841 | 1.00 | 0.00 H |
| ATOM | 1307 2 | 2HB | PRO A | 89135.305 | 0.060 | 2.641 | 1.00 | 0.00 H |
| ATOM | 1308 | HG | PRO A | 89134.037 | 0.140 | 0.301 | 1.00 | 0.00 H |
| ATOM | 1309 2 | 2HG | PRO A | 89135.366 | 1.260 | 0.658 | 1.00 | 0.00 H |
| ATOM | 1310 | HD | PRO A | 89135.351 | -1.180 | -1.064 | 1.00 | 0.00 H |
| ATOM | 1311 2 | 2HD | PRO A | 89136.206 | 0.358 | -1.292 | 1.00 | 0.00 H |
| ATOM | 1312 | N | ASPA | 90137.960 | -2.426 | 3.190 | 1.00 | 0.00 N |
| ATOM | 1313 | CA | ASPA | 90138.264 | -3.694 | 3.844 | 1.00 | 0.00 C |
| ATOM | 1314 | C | ASPA | 90137.542 | -3.802 | 5.183 | 1.00 | 0.00 C |
| ATOM | 1315 | O | ASPA | 90137.962 | -3.209 | 6.176 | 1.00 | 0.00 O |
| ATOM | 1316 | CB | ASPA | 90139.773 | -3.835 | 4.052 | 1.00 | 0.00 C |
| ATOM | 1317 | CG | ASPA | 90140.201 | -5.279 | 4.220 | 1.00 | 0.00 C |
| ATOM | 1318 | OD1 | ASPA | 90140.849 | -5.592 | 5.241 | 1.00 | 0.00 O |
| ATOM | 1319 | OD2 | ASPA | 90139.886 | -6.098 | 3.331 | 1.00 | 0.00 O |
| ATOM | 1320 | Н | ASPA | 90138.399 | -1.609 | 3.505 | 1.00 | 0.00 H |
| ATOM | 1321 | HA | ASPA | 90137.923 | -4.488 | 3.199 | 1.00 | 0.00 H |
| ATOM | 1322 | lНВ | ASPA | 90140.288 | -3.423 | 3.197 | 1.00 | 0.00 H |
| ATOM | 1323 | 2HB | ASPA | 90140.061 | -3.287 | 4.937 | 1.00 | 0.00 H |
| ATOM | 1324 | N | SER A | 91136.454 | - 4.564 | 5.202 | 1.00 | 0.00 N |
| ATOM | 1325 | CA | SER A | 91135.673 | -4.751 | 6.420 | 1.00 | 0.00 C |
| ATOM | 1326 | C | SER A | 91136.034 | -6.066 | 7.101 | 1.00 | 0.00°C |

| ATOM | 1327 | O | SER A | 91135.196 | -6.689 | 7.753 | 1.00 | 0.00 O |
|------|--------|-----|-------|-----------|---------|-------|------|--------|
| ATOM | 1328 | CB | SER A | 91134.177 | -4.723 | 6.101 | 1.00 | 0.00 C |
| ATOM | 1329 | OG | SER A | 91133.431 | -4.222 | 7.197 | 1.00 | 0.00 O |
| ATOM | 1330 | Н | SER A | 91136.168 | -5.012 | 4.378 | 1.00 | 0.00 H |
| ATOM | 1331 | НА | SER A | 91135.904 | -3.937 | 7.090 | 1.00 | 0.00 H |
| ATOM | 1332 1 | IHB | SER A | 91134.005 | -4.088 | 5.245 | 1.00 | 0.00 H |
| ATOM | 1333 2 | 2HB | SER A | 91133.841 | -5.725 | 5.881 | 1.00 | 0.00 H |
| ATOM | 1334 | HG | SER A | 91133.583 | -3.278 | 7.284 | 1.00 | 0.00 H |
| ATOM | 1335 | N | ARG A | 92137.285 | -6.486 | 6.944 | 1.00 | 0.00 N |
| ATOM | 1336 | CA | ARG A | 92137.756 | -7.728 | 7.544 | 1.00 | 0.00 C |
| ATOM | 1337 | C | ARG A | 92137.792 | -7.619 | 9.064 | 1.00 | 0.00 C |
| ATOM | 1338 | O | ARG A | 92137.609 | -8.610 | 9.772 | 1.00 | 0.00 O |
| ATOM | 1339 | СВ | ARG A | 92139.148 | -8.079 | 7.013 | 1.00 | 0.00 C |
| ATOM | 1340 | CG | ARG A | 92139.143 | -8.589 | 5.580 | 1.00 | 0.00 C |
| ATOM | 1341 | CD | ARG A | 92139.469 | -10.073 | 5.512 | 1.00 | 0.00 C |
| ATOM | 1342 | NE | ARG A | 92138.336 | -10.902 | 5.917 | 1.00 | 0.00 N |
| ATOM | 1343 | CZ | ARG A | 92138.226 | -12.197 | 5.630 | 1.00 | 0.00 C |
| ATOM | 1344 | NH1 | ARG A | 92139.176 | -12.813 | 4.938 | 1.00 | 0.00 N |
| ATOM | 1345 | NH2 | ARG A | 92137.162 | -12.877 | 6.034 | 1.00 | 0.00 N |
| ATOM | 1346 | Н | ARG A | 92137.907 | -5.946 | 6.412 | 1.00 | 0.00 H |
| ATOM | 1347 | НА | ARG A | 92137.067 | -8.511 | 7.267 | 1.00 | 0.00 H |
| ATOM | 1348 1 | lНВ | ARG A | 92139.770 | -7.197 | 7.057 | 1.00 | 0.00 H |
| ATOM | 1349 2 | 2HB | ARG A | 92139.579 | -8.843 | 7.644 | 1.00 | 0.00 H |
| ATOM | 1350 1 | HG | ARG A | 92138.163 | -8.427 | 5.155 | 1.00 | 0.00 H |
| ATOM | 1351 2 | 2HG | ARG A | 92139.879 | -8.040 | 5.012 | 1.00 | 0.00 H |
| ATOM | 1352 1 | HD | ARG A | 92139.739 | -10.322 | 4.497 | 1.00 | 0.00 H |
| ATOM | 1353 2 | 2HD | ARG A | 92140.303 | -10.275 | 6.167 | 1.00 | 0.00 H |

| 1354 | HE | ARG A | 92137.620 - | -10.471 | 6.430 | 1.00 | 0.00 H |
|------|--|--|--|--|---|-----------------------------------|-----------------------------------|
| 1355 | 1HH1 A | ARG A | 92139.980 -1 | 12.307 | 4.629 | 1.00 | 0.00 H |
| 1356 | 2HH1 A | ARG A | 92139.088 -1 | 13.787 | 4.725 | 1.00 | 0.00 H |
| 1357 | 1HH2 / | ARG A | 92136.443 -1 | 12.418 | 6.556 | 1.00 | 0.00 H |
| 1358 | 2HH2 / | ARG A | 92137.079 - | 13.850 | 5.819 | 1.00 | 0.00 H |
| 1359 | N | PHE A | 93138.031 | -6.410 | 9.561 | 1.00 | 0.00 N |
| 1360 | CA | PHE A | 93138.092 | -6.172 | 10.999 | 1.00 | 0.00 C |
| 1361 | C | PHE A | 93136.976 | -5.233 | 11.447 | 1.00 | 0.00 C |
| 1362 | O | PHE A | 93137.114 | -4.519 | 12.440 | 1.00 | 0.00 O |
| 1363 | CB | PHE A | 93139.451 | -5.583 | 11.381 | 1.00 | 0.00 C |
| 1364 | CG | PHE A | 93140.586 | -6.559 | 11.253 | 1.00 | 0.00 C |
| 1365 | CD1 | PHE A | 93140.898 | -7.122 | 10.026 | 1.00 | 0.00 C |
| 1366 | CD2 | PHE A | 93141.340 | -6.914 | 12.361 | 1.00 | 0.00 C |
| 1367 | CE1 | PHE A | 93141.942 | -8.020 | 9.905 | 1.00 | 0.00 C |
| 1368 | CE2 | PHE A | 93142.385 | -7.811 | 12.246 | 1.00 | 0.00 C |
| 1369 | CZ | PHE A | 93142.686 | -8.365 . | 11.017 | 1.00 | 0.00 C |
| 1370 | Н | PHE A | 93138.170 | -5.659 | 8.947 | 1.00 | 0.00 H |
| 1371 | НА | PHE A | 93137.968 | -7.122 | 11.497 | 1.00 | 0.00 H |
| 1372 | 1HB | PHE A | 93139.664 | -4.741 | 10.740 | 1.00 | 0.00 H |
| 1373 | 2HB | PHE A | 93139.413 | -5.248 | 12.407 | 1.00 | 0.00 H |
| 1374 | HD1 | PHE A | 93140.317 | -6.853 | 9.156 | 1.00 | 0.00 H |
| 1375 | HD2 | PHE A | 93141.105 | -6.482 | 13.322 | 1.00 | 0.00 H |
| 1376 | HE1 | PHE A | 93142.175 | -8.451 | 8.944 | 1.00 | 0.00 H |
| 1377 | HE2 | PHE A | 93142.965 | -8.079 | 13.117 | 1.00 | 0.00 H |
| 1378 | HZ | PHE A | 93143.502 | -9.066 | 10.925 | 1.00 | 0.00 H |
| 1379 | N | ALA A | 94135.869 | -5.238 | 10.710 | 1.00 | 0.00 N |
| 1380 | CA | ALA A | 94134.732 | -4.386 | 11.038 | 1.00 | 0.00 C |
| | 1355 1356 1357 1358 1359 1360 1361 1362 1363 1364 1365 1366 1367 1368 1370 1371 1372 1373 1374 1375 1376 1377 | 1355 1HH1 A 1356 2HH1 A 1357 1HH2 A 1358 2HH2 A 1359 N 1360 CA 1361 C 1362 O 1363 CB 1364 CG 1365 CD1 1366 CD2 1367 CE1 1368 CE2 1369 CZ 1370 H 1371 HA 1372 1HB 1373 2HB 1374 HD1 1375 HD2 1376 HE1 1377 HE2 1378 HZ 1379 N | 1355 1HH1 ARG A 1356 2HH1 ARG A 1357 1HH2 ARG A 1358 2HH2 ARG A 1359 N PHE A 1360 CA PHE A 1361 C PHE A 1362 O PHE A 1364 CG PHE A 1365 CD1 PHE A 1366 CD2 PHE A 1367 CE1 PHE A 1368 CE2 PHE A 1369 CZ PHE A 1370 H PHE A 1371 HA PHE A 1371 HA PHE A 1372 1HB PHE A 1373 2HB PHE A 1373 HD1 PHE A 1374 HD1 PHE A 1375 HD2 PHE A 1376 HE1 PHE A 1377 HE2 PHE A | 1355 1HH1 ARG A 92139.980 - 1 1356 2HH1 ARG A 92139.088 - 1 1357 1HH2 ARG A 92136.443 - 1 1358 2HH2 ARG A 92137.079 - 1 1359 N PHE A 93138.031 1360 CA PHE A 93138.092 1361 C PHE A 93136.976 1362 O PHE A 93137.114 1363 CB PHE A 93139.451 1364 CG PHE A 93140.586 1365 CD1 PHE A 93140.898 1366 CD2 PHE A 93141.340 1367 CE1 PHE A 93141.340 1368 CE2 PHE A 93142.385 1369 CZ PHE A 93142.886 1370 H PHE A 93138.170 1371 HA PHE A 93139.664 1373 2HB PHE A 93139.664 1373 2HB PHE A 93139.413 1374 HD1 PHE A 93140.317 1375 HD2 PHE A 93142.175 1376 HE1 PHE A 93142.965 1378 HZ PHE A 93143.502 1379 N ALAA 94135.869 | 1355 1HH1 ARG A 92139.980 -12.307 1356 2HH1 ARG A 92139.088 -13.787 1357 1HH2 ARG A 92137.079 -13.850 1358 2HH2 ARG A 92137.079 -13.850 1359 N PHE A 93138.031 -6.410 1360 CA PHE A 93138.092 -6.172 1361 C PHE A 93136.976 -5.233 1362 O PHE A 93137.114 -4.519 1363 CB PHE A 93139.451 -5.583 1364 CG PHE A 93140.586 -6.559 1365 CD1 PHE A 93140.898 -7.122 1366 CD2 PHE A 93141.340 -6.914 1367 CE1 PHE A 93141.942 -8.020 1368 CE2 PHE A 93142.385 -7.811 1369 CZ PHE A 93142.385 -7.811 1369 CZ PHE A 93139.466 -8.365 . 1370 H PHE A 93139.666 -8.365 . 1371 HA PHE A 93139.664 -4.741 1373 2HB PHE A 93139.664 -4.741 1373 2HB PHE A 93139.413 -5.248 1374 HD1 PHE A 93140.317 -6.853 1375 HD2 PHE A 93142.175 -8.451 1377 HE2 PHE A 93142.965 -8.079 1378 HZ PHE A 93143.502 -9.066 1379 N ALAA 94135.869 -5.238 | 1355 1HH1 ARG A 92139.980 -12.307 | 1355 1HH1 ARG A 92139.980 -12.307 |

| ATOM | 1381 | C . | ALA A | 94133.628 | -5.181 | 11.726 | 1.00 | 0.00 C |
|--------|--------|-----|-------|-----------|--------|--------|------|--------|
| ATOM | 1382 | O | ALA A | 94133.159 | -6.193 | 11.204 | 1.00 | 0.00 O |
| ATOM | 1383 | CB | ALA A | 94134.197 | -3.716 | 9.780 | 1.00 | 0.00 C |
| ATOM | 1384 | Н | ALA A | 94135.814 | -5.829 | 9.930 | 1.00 | 0.00 H |
| ATOM | 1385 | НА | ALA A | 94135.077 | -3.614 | 11.709 | 1.00 | 0.00 H |
| ATOM | 1386 1 | НВ | ALA A | 94133.322 | -4.246 | 9.434 | 1.00 | 0.00 H |
| ATOM | 1387 2 | 2HB | ALA A | 94134.956 | -3.732 | 9.013 | 1.00 | 0.00 H |
| ATOM | 1388 3 | BHB | ALA A | 94133.932 | -2.693 | 10.004 | 1.00 | 0.00 H |
| ATOM · | 1389 | N | SER A | 95133.216 | -4.717 | 12.902 | 1.00 | 0.00 N |
| ATOM | 1390 | CA | SER A | 95132.167 | -5.384 | 13.663 | 1.00 | 0.00 C |
| ATOM | 1391 | C | SER A | 95130.804 | -4.767 | 13.363 | 1.00 | 0.00 C |
| ATOM | 1392 | O | SER A | 95130.659 | -3.546 | 13.331 | 1.00 | 0.00 O |
| ATOM | 1393 | CB | SER A | 95132.460 | -5.298 | 15.162 | 1.00 | 0.00 C |
| ATOM | 1394 | OG | SER A | 95133.403 | -6.280 | 15.554 | 1.00 | 0.00 O |
| ATOM | 1395 | Н | SER A | 95133.629 | -3.905 | 13.266 | 1.00 | 0.00 H |
| ATOM | 1396 | НА | SER A | 95132.152 | -6.422 | 13.366 | 1.00 | 0.00 H |
| ATOM | 1397 | HB | SER A | 95132.860 | -4.322 | 15.392 | 1.00 | 0.00 H |
| ATOM | 1398 2 | 2HB | SER A | 95131.546 | -5.452 | 15.714 | 1.00 | 0.00 H |
| ATOM | 1399 | HG | SER A | 95132.941 | -7.050 | 15.894 | 1.00 | 0.00 H |
| ATOM | 1400 | N | LEU A | 96129.809 | -5.620 | 13.143 | 1.00 | 0.00 N |
| ATOM | 1401 | CA | LEU A | 96128.459 | -5.157 | 12.847 | 1.00 | 0.00 C |
| ATOM | 1402 | C | LEU A | 96127.448 | -6.288 | 13.000 | 1.00 | 0.00 C |
| ATOM | 1403 | O | LEU A | 96127.601 | -7.357 | 12.405 | 1.00 | 0.00 O |
| ATOM | 1404 | CB | LEU A | 96128.394 | -4.589 | 11.428 | 1.00 | 0.00 C |
| ATOM | 1405 | CG | LEU A | 96127.019 | -4.076 | 10.997 | 1.00 | 0.00 C |
| ATOM | 1406 | CD1 | LEU A | 96126.635 | -2.843 | 11.801 | 1.00 | 0.00 C |
| ATOM | 1407 | CD2 | LEU A | 96127.009 | -3.769 | 9.507 | 1.00 | 0.00 C |

ATOM 1408 Η LEU A 96129.987 0.00 H-6.583 13.183 1.00 **ATOM** 1409 HA LEUA 96128.215 -4.375 13.549 1.00 0.00 H**ATOM** 1410 1HB LEUA 96129.099 -3.773 11.358 1.00 0.00 H**ATOM** LEU A 1.00 1411 2HB 96128.696 -5.363 10.738 0.00 H 1412 HG LEUA 96126.281 1.00 0.00 H **ATOM** -4.841 11.187 **ATOM** 1413 1HD1 LEU A 96126.375 -3.136 12.807 1.00 0.00 H1414 2HD1 LEU A 1.00 0.00 H**ATOM** 96125.788 -2.360 11.336 1415 3HD1 LEU A 96127.468 1.00 **ATOM** -2.157 11.829 0.00 H1416 1HD2 LEU A 96127.887 -3.195 1.00 0.00 H **ATOM** 9.252 1417 2HD2 LEU A 96126.124 1.00 0.00 H**ATOM** -3.200 9.263 **ATOM** 1418 3HD2 LEU A 96127.008 -4.693 8.949 1.00 0.00 H **ATOM** 1419 N GLN A 97126.414 -6.047 13.800 1.00 0.00 N 97125.375 -7.044 14.031 1.00 0.00 C **ATOM** 1420 CA GLNA **ATOM** 1421 C GLN A 97124.046 -6.595 13.432 1.00 0.00 C 97123.770 -5.398 13.339 1.00 0.00 O **ATOM** 1422 0 GLN A GLN A 97125.212 -7.303 15.529 1.00 0.00 C **ATOM** 1423 CB97126.300 -8.185 16.117 1.00 0.00 C **ATOM** 1424 CG GLN A **ATOM** 1425 CD GLN A 97126.152 -9.640 15.720 1.00 0.00 C 1426 97125.213 -10.317 16.141 1.00 0.00 O**ATOM** OE1 GLN A 1.00 97127.077 -10.129 14.903 0.00 N **ATOM** 1427 NE2 GLN A 97126.347 -5.176 14.244 1.00 0.00 H **ATOM** 1428 Η GLN A 13.548 **ATOM** 1429 HA GLNA 97125.682 -7.961 1.00 0.00 H 16.050 1.00 1430 1HB GLN A 97125.225 -6.356 0.00 H **ATOM** 15.699 1.00 0.00 H **ATOM** 1431 2HB GLN A 97124.259 -7.784 15.771 1.00 0.00 H **ATOM** - 1432 1HG GLN A 97127.260 -7.830 17.196 1.00 97126.260 -8.115 0.00 H**ATOM** 1433 2HG GLN A 97127.796 -9.531 14.608 1.00 0.00 H **ATOM** 1434 1HE2 GLN A

| ATOM | 1435 | 2HE2 | GLN A | 97127.005 - | 11.066 | 14.630 | 1.00 | 0.00 H |
|--------|------|------|-------|-------------|---------|--------|------|--------|
| ATOM | 1436 | N | PRO A | 98123.198 | -7.552 | 13.015 | 1.00 | 0.00 N |
| ATOM | 1437 | CA | PRO A | 98121.892 | -7.248 | 12.423 | 1.00 | 0.00 C |
| ATOM | 1438 | C | PRO A | 98121.064 | -6.310 | 13.296 | 1.00 | 0.00 C |
| ATOM | 1439 | O | PRO A | 98121.520 | -5.859 | 14.346 | 1.00 | 0.00 O |
| ATOM | 1440 | СВ | PRO A | 98121.218 | -8.617 | 12.320 | 1.00 | 0.00 C |
| ATOM | 1441 | CG | PRO A | 98122.345 | -9.589 | 12.252 | 1.00 | 0.00 C |
| ATOM 🐛 | 1442 | CD | PRO A | 98123.448 | -9.004 | 13.089 | 1.00 | 0.00 C |
| ATOM | 1443 | НА | PRO A | 98121.996 | -6.819 | 11.436 | 1.00 | 0.00 H |
| ATOM | 1444 | 1HB | PRO A | 98120.603 | -8.785 | 13.193 | 1.00 | 0.00 H |
| ATOM | 1445 | 2HB | PRO A | 98120.610 | -8.657 | 11.430 | 1.00 | 0.00 H |
| ATOM | 1446 | 1HG | PRO A | 98122.033 | -10.541 | 12.655 | 1.00 | 0.00 H |
| ATOM | 1447 | 2HG | PRO A | 98122.671 | -9.702 | 11.228 | 1.00 | 0.00 H |
| ATOM | 1448 | 1HD | PRO A | 98123.376 | -9.356 | 14.108 | 1.00 | 0.00 H |
| ATOM | 1449 | 2HD | PRO A | 98124.412 | -9.251 | 12.670 | 1.00 | 0.00 H |
| ATOM | 1450 | N | SER A | 99119.844 | -6.023 | 12.855 | 1.00 | 0.00 N |
| ATOM | 1451 | CA | SER A | 99118.951 | -5.140 | 13.597 | 1.00 | 0.00 C |
| ATOM | 1452 | C | SER A | 99117.810 | - 5.928 | 14.232 | 1.00 | 0.00 C |
| ATOM - | 1453 | O | SER A | 99117.697 | -5.997 | 15.456 | 1.00 | 0.00 O |
| ATOM | 1454 | СВ | SER A | 99118.386 | -4.058 | 12.675 | 1.00 | 0.00 C |
| ATOM | 1455 | OG | SER A | 99118.327 | -4.512 | 11.333 | 1.00 | 0.00 O |
| ATOM | 1456 | Н | SER A | 99119.535 | -6.414 | 12.011 | 1.00 | 0.00 H |
| ATOM | 1457 | НА | SER A | 99119.527 | -4.669 | 14.379 | 1.00 | 0.00 H |
| ATOM | 1458 | 1HB | SER A | 99117.390 | -3.797 | 12.997 | 1.00 | 0.00 H |
| ATOM | 1459 | 2HB | SER A | 99119.020 | -3.184 | 12.717 | 1.00 | 0.00 H |
| ATOM | 1460 | HG | SER A | 99118.412 | -3.764 | 10.737 | 1.00 | 0.00 H |
| ATOM | 1461 | N | GLY A | 100116.966 | -6.519 | 13.393 | 1.00 | 0.00 N |

| ATOM | 1462 | CA | GLY A 100115.846 | -7.293 | 13.892 | 1.00 | 0.00 C |
|------|--------|-----|------------------|--------|--------|--------|--------|
| ATOM | 1463 | C | GLY A 100114.524 | -6.565 | 13.742 | 1.00 | 0.00 C |
| ATOM | 1464 | О | GLY A 100114.144 | -5.782 | 14.613 | 1.00 | 0.00 O |
| ATOM | 1465 | Н | GLY A 100117.107 | -6.428 | 12.427 | 1.00 | 0.00 H |
| ATOM | 1466 | НА | GLY A 100115.796 | -8.225 | 13.347 | 1.00 | 0.00 H |
| ATOM | 1467 2 | 2HA | GLY A 100116.009 | -7.509 | 14.937 | 1.00 | 0.00 H |
| ATOM | 1468 | N | PRO A 101113.793 | -6.802 | 12.638 | 1.00 | 0.00 N |
| ATOM | 1469 | CA | PRO A 101112.500 | -6.153 | 12.392 | 1.00 | 0.00 C |
| ATOM | 1470 | C | PRO A 101111.553 | -6.277 | 13.581 | 1.00 | 0.00 C |
| ATOM | 1471 | O | PRO A 101111.276 | -7.378 | 14.055 | 1.00 | 0.00 O |
| ATOM | 1472 | СВ | PRO A 101111.946 | -6.912 | 11.186 | 1.00 | 0.00 C |
| ATOM | 1473 | CG | PRO A 101113.151 | -7.427 | 10.478 | 1.00 | 0.00 C |
| ATOM | 1474 | CD | PRO A 101114.167 | -7.720 | 11.546 | 1.00 | 0.00 C |
| ATOM | 1475 | НА | PRO A 101112.624 | -5.110 | 12.139 | 1.00 | 0.00 H |
| ATOM | 1476 | lНВ | PRO A 101111.311 | -7.718 | 11.525 | 1.00 | 0.00 H |
| ATOM | 1477 2 | 2HB | PRO A 101111.380 | -6.238 | 10.561 | 1.00 | 0.00 H |
| ATOM | 1478 | HG | PRO A 101112.901 | -8.329 | 9.939 | 1.00 | 0.00 H |
| ATOM | 1479 2 | 2HG | PRO A 101113.526 | -6.676 | 9.799 | 1.00 | 0.00 H |
| ATOM | 1480 | IHD | PRO A 101114.093 | -8.749 | 11.865 | 1.00 | 0.00 H |
| ATOM | 1481 2 | 2HD | PRO A 101115.164 | -7.505 | 11.188 | 1.00 | 0.00 H |
| ATOM | 1482 | N | SER A 102111.061 | -5.138 | 14.060 | 1.00 | 0.00 N |
| ATOM | 1483 | CA | SER A 102110.144 | -5.120 | 15.194 | 1.00 | 0.00 C |
| ATOM | 1484 | C | SER A 102110.802 | -5.719 | 16.434 | 1.00 | 0.00 C |
| ATOM | 1485 | O | SER A 102110.493 | -6.842 | 16.831 | 1.00 | 0.00 O |
| ATOM | 1486 | СВ | SER A 102108.866 | -5.890 | 14.857 | 1.00 | 0.00 C |
| ATOM | 1487 | OG | SER A 102107.873 | -5.024 | 14.333 | · 1.00 | 0.00 O |
| ATOM | 1488 | Н | SER A 102111.319 | -4.292 | 13.640 | 1.00 | 0.00 H |

| ATOM | 1489 HA | SER A 102109.891 | -4.091 | 15.398 | 1.00 | 0.00 H |
|------|------------|--------------------|--------|--------|------|--------|
| ATOM | 1490 1HB | SER A 102109.088 | -6.647 | 14.120 | 1.00 | 0.00 H |
| ATOM | 1491 2HB | SER A 102108.483 | -6.358 | 15.752 | 1.00 | 0.00 H |
| ATOM | 1492 HG | SER A 102108.270 | -4.434 | 13.690 | 1.00 | 0.00 H |
| ATOM | 1493 N | SER A 103111.709 | -4.961 | 17.041 | 1.00 | 0.00 N |
| ATOM | 1494 CA | SER A 103112.410 | -5.416 | 18.235 | 1.00 | 0.00 C |
| ATOM | 1495 C | SER A 103111.554 | -5.208 | 19.481 | 1.00 | 0.00 C |
| ATOM | 1496 O | SER A 103110.663 | -4.359 | 19.498 | 1.00 | 0.00 O |
| ATOM | 1497 CB | SER A 103113.740 | -4.676 | 18.385 | 1.00 | 0.00 C |
| ATOM | 1498 OG | SER A 103114.772 | -5.329 | 17.666 | 1.00 | 0.00 O |
| ATOM | 1499 H | SER A 103111.912 | -4.075 | 16.676 | 1.00 | 0.00 H |
| ATOM | 1500 HA | SER A 103112.607 | -6.472 | 18.121 | 1.00 | 0.00 H |
| ATOM | 1501 1HB | SER A 103113.634 | -3.670 | 18.006 | 1.00 | 0.00 H |
| ATOM | 1502 2HB | SER A 103114.013 | -4.638 | 19.430 | 1.00 | 0.00 H |
| ATOM | 1503 HG | SER A 103114.839 | -6.240 | 17.960 | 1.00 | 0.00 H |
| ATOM | 1504 N | GLY A 104111.832 | -5.986 | 20.520 | 1.00 | 0.00 N |
| ATOM | 1505 CA | GLY A 104111.079 | -5.871 | 21.756 | 1.00 | 0.00 C |
| ATOM | 1506 C | GLY A 104111.969 | -5.896 | 22.983 | 1.00 | 0.00 C |
| ATOM | 1507 O | GLY A 104111.575 | -6.523 | 23.989 | 1.00 | 0.00 O |
| ATOM | 1508 OX | T GLY A 104113.061 | -5.291 | 22.937 | 1.00 | 0.00 O |
| ATOM | 1509 H | GLY A 104112.555 | -6.645 | 20.449 | 1.00 | 0.00 H |
| ATOM | 1510 1HA | GLY A 104110.529 | -4.941 | 21.743 | 1.00 | 0.00 H |
| ATOM | 1511 2HA | GLY A 104110.379 | -6.691 | 21.815 | 1.00 | 0.00 H |
| TER | 1512 GLY A | . 104 | | | | |

ENDMDL

Three-Dimensional Structure Coordinate Table 10

| ATOM 1 | N | GLY A | 1132.485 | -2.135 -1 | 14.848 | 1.00 | 0.00 N |
|----------|-----|--------|----------|-----------|---------|------|--------|
| ATOM 2 | CA | GLY A | 1133.474 | -2.831 - | 13.979 | 1.00 | 0.00 C |
| ATOM 3 | C | GLY A | 1133.260 | -2.538 -1 | 2.507 | 1.00 | 0.00·C |
| ATOM 4 | О | GLY A | 1133.286 | -3.446 - | 11.676 | 1.00 | 0.00 O |
| ATOM 5 1 | Н | GLY A | 1132.906 | -1.268 -1 | 5.244 | 1.00 | 0.00 H |
| ATOM 6 2 | Н | GLY A | 1131.643 | -1.877 -1 | 4.296 | 1.00 | 0.00 H |
| ATOM 7 3 | Н | GLY A | 1132.197 | -2.756 -1 | 5.631 | 1.00 | 0.00 H |
| ATOM 8 1 | HA | GLY A | 1133.389 | -3.896 -1 | 4.138 | 1.00 | 0.00 H |
| ATOM 9 2 | HA | GLY A | 1134.468 | -2.515 -1 | 4.257 | 1.00 | 0.00 H |
| ATOM10 | N | SER A | 2133.048 | -1.266 - | 12.184 | 1.00 | 0.00 N |
| ATOM11 | CA | SER A | 2132.829 | -0.855 - | 10.803 | 1.00 | 0.00 C |
| ATOM12 | C | SER A | 2131.367 | -0.493 - | 10.568 | 1.00 | 0.00 C |
| ATOM13 | O | SER A | 2130.763 | 0.238 - | 11.354 | 1.00 | 0.00 O |
| ATOM14 | CB | SER A | 2133.723 | 0.338 | -10.456 | 1.00 | 0.00 C |
| ATOM15 | OG | SER A | 2133.256 | 1.523 | -11.074 | 1.00 | 0.00 O |
| ATOM16 | Н | SER A | 2133.039 | -0.588 - | 12.892 | 1.00 | 0.00 H |
| ATOM17 | НА | SER A | 2133.089 | -1.686 - | 10.164 | 1.00 | 0.00 H |
| ATOM18 | lНВ | SER A | 2133.727 | 0.483 | -9.386 | 1.00 | 0.00 H |
| ATOM19 2 | 2HB | SER A | 2134.729 | 0.141 - | 10.795 | 1.00 | 0.00 H |
| ATOM20 | HG | SER A | 2133.668 | 2.285 | -10.661 | 1.00 | 0.00 H |
| ATOM21 | N | SER A | 3130.801 | -1.010 | -9.482 | 1.00 | 0.00 N |
| ATOM22 | CA | SER A | 3129.408 | -0.742 | -9.143 | 1.00 | 0.00 C |
| ATOM23 | C | SER A | 3129.287 | 0.525 | -8.303 | 1.00 | 0.00 C |
| ATOM24 | Ο | SER A | 3129.369 | 0.478 | -7.076 | 1.00 | 0.00 O |
| ATOM25 | CB | SER A | 3128.807 | -1.928 | -8.388 | 1.00 | 0.00 C |
| ATOM26 | OG | SER A | 3127.458 | -2.142 | -8.764 | 1.00 | 0.00 O |
| ATOM27 | Н | ·SER A | 3131.334 | -1.586 | -8.893 | 1.00 | 0.00 H |

| ATOM28 | НА | SER A | 3128.865 | -0.602 - | 10.066 | 1.00 | 0.00 H |
|--------|-----|-------|----------|----------|---------|------|--------|
| ATOM29 | 1HB | SER A | 3129.375 | -2.820 | -8.612 | 1.00 | 0.00 H |
| ATOM30 | 2HB | SER A | 3128.847 | -1.734 | -7.326 | 1.00 | 0.00 H |
| ATOM31 | HG | SER A | 3126.975 | -1.313 | -8.709 | 1.00 | 0.00 H |
| ATOM32 | N | GLY A | 4129.091 | 1.657 | -8.972 | 1.00 | 0.00 N |
| ATOM33 | CA | GLY A | 4128.962 | 2.919 | -8.271 | 1.00 | 0.00 C |
| ATOM34 | C | GLY A | 4128.420 | 4.023 | -9.158 | 1.00 | 0.00 C |
| ATOM35 | Ο | GLY A | 4128.458 | 3.918 | -10.383 | 1.00 | 0.00 O |
| ATOM36 | Н | GLY A | 4129.035 | 1.633 | -9.950 | 1.00 | 0.00 H |
| ATOM37 | 1HA | GLY A | 4128.293 | 2.787 | -7.432 | 1.00 | 0.00 H |
| ATOM38 | 2HA | GLY A | 4129.932 | 3.214 | -7.901 | 1.00 | 0.00 H |
| ATOM39 | N | SER A | 5127.915 | 5.084 | -8.537 | 1.00 | 0.00 N |
| ATOM40 | CA | SER A | 5127.362 | 6.212 | -9.279 | 1.00 | 0.00 C |
| ATOM41 | C | SER A | 5127.409 | 7.487 | -8.444 | 1.00 | 0.00 C |
| ATOM42 | Ο | SER A | 5127.856 | 8.534 | -8.914 | 1.00 | 0.00 O |
| ATOM43 | CB | SER A | 5125.922 | 5.916 | -9.699 | 1.00 | 0.00 C |
| ATOM44 | OG | SER A | 5125.076 | 5.793 | -8.569 | 1.00 | 0.00 O |
| ATOM45 | Н | SER A | 5127.913 | 5.110 | -7.558 | 1.00 | 0.00 H |
| ATOM46 | HA | SER A | 5127.964 | 6.353 | -10.164 | 1.00 | 0.00 H |
| ATOM47 | 1HB | SER A | 5125.558 | 6.722 - | 10.319 | 1.00 | 0.00 H |
| ATOM48 | 2HB | SER A | 5125.895 | 4.993 - | 10.258 | 1.00 | 0.00 H |
| ATOM49 | HG | SER A | 5124.212 | 6.159 | -8.774 | 1.00 | 0.00 H |
| ATOM50 | N | SER A | 6126.945 | 7.394 | -7.202 | 1.00 | 0.00 N |
| ATOM51 | CA | SER A | 6126.933 | 8.540 | -6.301 | 1.00 | 0.00 C |
| ATOM52 | C | SER A | 6128.282 | 8.699 | -5.606 | 1.00 | 0.00 C |
| ATOM53 | О | SER A | 6129.041 | 7.739 | -5.475 | 1.00 | 0.00 O |
| ATOM54 | СВ | SER A | 6125.824 | 8.385 | -5.259 | 1.00 | 0.00 C |

| ATOM55 | OG | SER A | 6125.843 | 7.091 | -4.683 | 1.00 | 0.00 O |
|--------|------|-------|----------|--------|--------|------|--------|
| ATOM56 | Н | SER A | 6126.601 | 6.532 | -6.884 | 1.00 | 0.00 H |
| ATOM57 | НА | SER A | 6126.740 | 9.423 | -6.892 | 1.00 | 0.00 H |
| ATOM58 | 1HB | SER A | 6125.965 | 9.115 | -4.475 | 1.00 | 0.00 H |
| ATOM59 | 2HB | SER A | 6124.866 | 8.543 | -5.731 | 1.00 | 0.00 H |
| ATOM60 | HG | SER A | 6126.724 | 6.899 | -4.353 | 1.00 | 0.00 H |
| ATOM61 | N | GLY A | 7128.574 | 9.917 | -5.163 | 1.00 | 0.00 N |
| ATOM62 | CA | GLY A | 7129.830 | 10.179 | -4.487 | 1.00 | 0.00 C |
| ATOM63 | C | GLY A | 7129.885 | 11.568 | -3.882 | 1.00 | 0.00 C |
| ATOM64 | О | GLY A | 7130.880 | 12.278 | -4.029 | 1.00 | 0.00 O |
| ATOM65 | Н | GLY A | 7127.930 | 10.645 | -5.297 | 1.00 | 0.00 H |
| ATOM66 | 1HA | GLY A | 7129.962 | 9.451 | -3.702 | 1.00 | 0.00 H |
| ATOM67 | 2HA | GLY A | 7130.637 | 10.078 | -5.198 | 1.00 | 0.00 H |
| ATOM68 | N | LEU A | 8128.813 | 11.957 | -3.200 | 1.00 | 0.00 N |
| ATOM69 | CA | LEU A | 8128.741 | 13.271 | -2.570 | 1.00 | 0.00 C |
| ATOM70 | C | LEU A | 8128.749 | 13.146 | -1.050 | 1.00 | 0.00 C |
| ATOM71 | О | LEU A | 8128.123 | 13.940 | -0.349 | 1.00 | 0.00 O |
| ATOM72 | CB | LEU A | 8127.482 | 14.011 | -3.026 | 1.00 | 0.00 C |
| ATOM73 | CG | LEU A | 8127.632 | 14.802 | -4.326 | 1.00 | 0.00 C |
| ATOM74 | CD1 | LEU A | 8126.291 | 14.925 | -5.034 | 1.00 | 0.00 C |
| ATOM75 | CD2 | LEU A | 8128.217 | 16.179 | -4.047 | 1.00 | 0.00 C |
| ATOM76 | Н | LEU A | 8128.050 | 11.347 | -3.119 | 1.00 | 0.00 H |
| ATOM77 | НА | LEU A | 8129.610 | 13.834 | -2.878 | 1.00 | 0.00 H |
| ATOM78 | 1HB | LEU A | 8126.692 | 13.286 | -3.158 | 1.00 | 0.00 H |
| ATOM79 | 2HB | LEU A | 8127.190 | 14.697 | -2.245 | 1.00 | 0.00 H |
| ATOM80 | HG | LEU A | 8128.308 | 14.277 | -4.983 | 1.00 | 0.00 H |
| ATOM81 | 1HD1 | LEU A | 8126.239 | 15.875 | -5.546 | 1.00 | 0.00 H |

ATOM82 2HD1 LEU A 8125.493 14.863 -4.307 1.00 0.00 HATOM83 3HD1 LEU A 8126.187 14.124 -5.750 1.00 0.00 HATOM84 1HD2 LEU A 8127.824 16.888 -4.760 1.00 0.00 H ATOM85 2HD2 LEU A 8129.293 16.137 -4.136 1.00 0.00 H ATOM86 3HD2 LEU A 8127.950 16.487 -3.047 1.00 0.00 H ATOM87 N **ALAA** 9129.465 12.144 -0.548 1.00 0.00 N ATOM88 CA ALAA 9129.555 11.916 0.889 1.00 0.00 C ATOM89 C 9130.916 11.341 1.267 1.00 0.00 C ALA A ATOM90 О **ALAA** 9131.007 10.386 2.039 1.00 0.00 O ATOM91 9128.440 10.988 1.346 1.00 0.00 C CB ALA A ATOM92 Η ALA A 9129.942 11.546 -1.158 1.00 0.00 H HA ALAA ATOM93 9129.426 12.866 1.386 1.00 0.00 H ATOM94 1HB ALA A 9128.296 11.095 2.411 1.00 0.00 HATOM95 2HB ALA A 9128.707 9.966 1.120 1.00 0.00 H ATOM96 3HB 9127.526 11.242 0.831 1.00 0.00 HALA A ATOM97 N 10131.974 11.929 0.717 1.00 0.00 N MET A ATOM98 10133.332 11.475 0.996 1.00 0.00 C CA MET A 0.00 C ATOM99 \mathbf{C} MET A 10134.283 12.661 1.158 1.00 **ATOM** 100 О MET A 10135.242 12.808 0.401 1.00 0.00 O 10133.825 1.00 0.00 C **ATOM** 101 CB MET A 10.557 -0.127 10133.494 11.064 -1.523 1.00 0.00 C 102 CG **MET A ATOM** 10134.899 11.857 -2.329 1.00 0.00 S **ATOM** 103 SD MET A 10134.803 11.137 -3.965 1.00 0.00 C **ATOM** 104 CE MET A 10131.838 12.686 0.109 1.00 0.00 H**ATOM** 105 Η MET A 10.918 1.920 1.00 0.00 H **ATOM** 106 HA META 10133.311 -0.0481.00 0.00 H107 1HB MET A 10134.897 10.458 **ATOM ATOM** 108 2HB MET A 10133.372 9.584 -0.004 1.00 0.00 H

| ATOM | 109 1HG | MET A | 10133.178 | 10.227 | -2.128 | 1.00 | 0.00 H |
|------|---------|-------|-----------|--------|--------|------|--------|
| ATOM | 110 2HG | MET A | 10132.687 | 11.778 | -1.452 | 1.00 | 0.00 H |
| ATOM | 111 1HE | MET A | 10135.673 | 11.424 | -4.536 | 1.00 | 0.00 H |
| ATOM | 112 2HE | MET A | 10133.912 | 11.489 | -4.462 | 1.00 | 0.00 H |
| ATOM | 113 3HE | MET A | 10134.767 | 10.060 | -3.883 | 1.00 | 0.00 H |
| ATOM | 114 N | PRO A | 11134.028 | 13.530 | 2.154 | 1.00 | 0.00 N |
| ATOM | 115 CA | PRO A | 11134.869 | 14.707 | 2.406 | 1.00 | 0.00 C |
| ATOM | 116 C | PRO A | 11136.323 | 14.343 | 2.706 | 1.00 | 0.00 C |
| ATOM | 117 O | PRO A | 11137.243 | 14.934 | 2.142 | 1.00 | 0.00 O |
| ATOM | 118 CB | PRO A | 11134.223 | 15.370 | 3.629 | 1.00 | 0.00 C |
| ATOM | 119 CG | PRO A | 11132.840 | 14.818 | 3.694 | 1.00 | 0.00 C |
| ATOM | 120 CD | PRO A | 11132.907 | 13.439 | 3.104 | 1.00 | 0.00 C |
| ATOM | 121 HA | PRO A | 11134.841 | 15.391 | 1.570 | 1.00 | 0.00 H |
| ATOM | 122 1HB | PRO A | 11134.789 | 15.125 | 4.514 | 1.00 | 0.00 H |
| ATOM | 123 2HB | PRO A | 11134.212 | 16.441 | 3.492 | 1.00 | 0.00 H |
| ATOM | 124 1HG | PRO A | 11132.515 | 14.768 | 4.723 | 1.00 | 0.00 H |
| ATOM | 125 2HG | PRO A | 11132.170 | 15.439 | 3.119 | 1.00 | 0.00 H |
| ATOM | 126 1HD | PRO A | 11133.108 | 12.708 | 3.873 | 1.00 | 0.00 H |
| ATOM | 127 2HD | PRO A | 11131.985 | 13.205 | 2.592 | 1.00 | 0.00 H |
| ATOM | 128 .N | PRO A | 12136.556 | 13.370 | 3.608 | 1.00 | 0.00 N |
| ATOM | 129 CA | PRO A | 12137.907 | 12.949 | 3.978 | 1.00 | 0.00 C |
| ATOM | 130 C | PRO A | 12138.499 | 11.939 | 3.000 | 1.00 | 0.00 C |
| ATOM | 131 O | PRO A | 12139.664 | 12.044 | 2.616 | 1.00 | 0.00 O |
| ATOM | 132 CB | PRO A | 12137.694 | 12.306 | 5.345 | 1.00 | 0.00 C |
| ATOM | 133 CG | PRO A | 12136.322 | 11.725 | 5.275 | 1.00 | 0.00 C |
| ATOM | 134 CD | PRO A | 12135.527 | 12.609 | 4.344 | 1.00 | 0.00 C |
| ATOM | 135 HA | PRO A | 12138.574 | 13.792 | 4.073 | 1.00 | 0.00 H |

| ATOM | 136 1HB | PRO A | 12138.441 | 11.543 | 5.507 | 1.00 | 0.00 H |
|------|---------------------|---------|-----------|--------|--------|------|--------|
| ATOM | 137 2HB | PRO A | 12137.765 | 13.059 | 6.116 | 1.00 | 0.00 H |
| ATOM | 138 1HG | PRO A | 12136.371 | 10.720 | 4.885 | 1.00 | 0.00 H |
| ATOM | 139 2HG | PRO A | 12135.876 | 11.724 | 6.259 | 1.00 | 0.00 H |
| ATOM | 140 1HD | PRO A | 12134.939 | 12.007 | 3.668 | 1.00 | 0.00 H |
| ATOM | 141 2HD | PRO A | 12134.889 | 13.271 | 4.910 | 1.00 | 0.00 H |
| ATOM | 142 N | GLY A | 13137.695 | 10.958 | 2.605 | 1.00 | 0.00 N |
| ATOM | 143 CA | GLY A | 13138.165 | 9.942 | 1.680 | 1.00 | 0.00 C |
| ATOM | 144 C | GLY A | 13137.387 | 9.927 | 0.380 | 1.00 | 0.00 C |
| ATOM | 145 O | GLY A | 13137.055 | 10.980 | -0.165 | 1.00 | 0.00 O |
| ATOM | 146 H | GLY A | 13136.776 | 10.921 | 2.947 | 1.00 | 0.00 H |
| ATOM | 147 1HA | GLY A | 13139.206 | 10.126 | 1.460 | 1.00 | 0.00 H |
| ATOM | 148 ₂ HA | GLY A | 13138.075 | 8.975 | 2.152 | 1.00 | 0.00 H |
| ATOM | 149 N | ASN A | 14137.097 | 8.729 | -0.117 | 1.00 | 0.00 N |
| ATOM | 150 CA | ASN A | 14136.354 | 8.576 | -1.364 | 1.00 | 0.00 C |
| ATOM | 151 C | ASN A | 14135.392 | 7.395 | -1.282 | 1.00 | 0.00 C |
| ATOM | 152 O | ASN A | 14135.721 | 6.353 | -0.716 | 1.00 | 0.00 O |
| ATOM | 153 CB | ASN A | 14137.318 | 8.384 | -2.536 | 1.00 | 0.00 C |
| ATOM | 154 CG | ASN A | 14138.440 | 9.403 | -2.536 | 1.00 | 0.00 C |
| ATOM | 155 OD: | I ASN A | 14138.425 | 10.362 | -3.307 | 1.00 | 0.00 O |
| ATOM | 156 ND2 | 2 ASN A | 14139.424 | 9.201 | -1.666 | 1.00 | 0.00 N |
| ATOM | 157 H | ASN A | 14137.390 | 7.928 | 0.364 | 1.00 | 0.00 H |
| ATOM | 158 HA | ASN A | 14135.785 | 9.479 | -1.523 | 1.00 | 0.00 H |
| ATOM | 159 1HB | ASN A | 14137.753 | 7.397 | -2.478 | 1.00 | 0.00 H |
| ATOM | 160 2HB | ASN A | 14136.771 | 8.478 | -3.462 | 1.00 | 0.00 H |
| ATOM | 161 1HD2 | ASN A | 14139.370 | 8.415 | -1.082 | 1.00 | 0.00 H |
| ATOM | 162 2HD2 | ASN A | 14140.162 | 9.844 | -1.644 | 1.00 | 0.00 H |

| ATOM | 163 | N | SER A | 15134.203 | 7.567 | -1.851 | 1.00 | 0.00 N |
|------|-------|-----|-------|-----------|-------|--------|------|--------|
| ATOM | 164 | CA | SER A | 15133.189 | 6.517 | -1.845 | 1.00 | 0.00 C |
| ATOM | 165 | C | SER A | 15132.729 | 6.212 | -0.422 | 1.00 | 0.00 C |
| ATOM | 166 | O | SER A | 15131.666 | 6.664 | 0.007 | 1.00 | 0.00 O |
| ATOM | 167 | СВ | SER A | 15133.733 | 5.247 | -2.504 | 1.00 | 0.00 C |
| ATOM | 168 | OG | SER A | 15133.356 | 5.179 | -3.869 | 1.00 | 0.00 O |
| ATOM | 169 | Н | SER A | 15134.001 | 8.422 | -2.287 | 1.00 | 0.00 H |
| ATOM | 170 | HA | SER A | 15132.344 | 6.872 | -2.414 | 1.00 | 0.00 H |
| ATOM | 171 | 1HB | SER A | 15134.811 | 5.244 | -2.442 | 1.00 | 0.00 H |
| ATOM | 172 2 | 2HB | SER A | 15133.341 | 4.381 | -1.991 | 1.00 | 0.00 H |
| ATOM | 173 | HG | SER A | 15132.415 | 5.352 | -3.950 | 1.00 | 0.00 H |
| ATOM | 174 | N | HIS A | 16133.533 | 5.445 | 0.306 | 1.00 | 0.00 N |
| ATOM | 175 | CA | HIS A | 16133.208 | 5.082 | 1.680 | 1.00 | 0.00 C |
| ATOM | 176 | C | HIS A | 16134.066 | 5.865 | 2.668 | 1.00 | 0.00 C |
| ATOM | 177 | O | HIS A | 16133.573 | 6.351 | 3.686 | 1.00 | 0.00 O |
| ATOM | 178 | CB | HIS A | 16133.405 | 3.580 | 1.894 | 1.00 | 0.00 C |
| ATOM | 179 | CG | HIS A | 16132.249 | 2.752 | 1.423 | 1.00 | 0.00 C |
| ATOM | 180 | ND1 | HIS A | 16131.753 | 1.680 | 2.135 | 1.00 | 0.00 N |
| ATOM | 181 | CD2 | HIS A | 16131.490 | 2.843 | 0.305 | 1.00 | 0.00 C |
| ATOM | 182 | CE1 | HIS A | 16130.739 | 1.148 | 1.475 | 1.00 | 0.00 C |
| ATOM | 183 | NE2 | HIS A | 16130.560 | 1.835 | 0.362 | 1.00 | 0.00 N |
| ATOM | 184 | Н | HIS A | 16134.367 | 5.115 | -0.090 | 1.00 | 0.00 H |
| ATOM | 185 | HA | HIS A | 16132.170 | 5.328 | 1.851 | 1.00 | 0.00 H |
| ATOM | 186 | 1HB | HIS A | 16134.284 | 3.260 | 1.355 | 1.00 | 0.00 H |
| ATOM | 187 | 2HB | HIS A | 16133.545 | 3.389 | 2.948 | 1.00 | 0.00 H |
| ATOM | 188 | HD1 | HIS A | 16132.093 | 1.357 | 2.995 | 1.00 | 0.00 H |
| ATOM | 189 | HD2 | HISA | 16131.598 | 3.573 | -0.485 | 1.00 | 0.00 H |

| ATOM | 190 | HE1 | HIS A | 16130.157 | 0.295 | 1.792 | 1.00 | 0.00 H | |
|------|-------|------|-------|-----------|-------|--------|------|--------|--|
| ATOM | 191 | HE2 | HIS A | 16129.823 | 1.704 | -0.270 | 1.00 | 0.00 H | |
| ATOM | 192 | N | GLY A | 17135.354 | 5.982 | 2.360 | 1.00 | 0.00 N | |
| ATOM | 193 | CA | GLY A | 17136.261 | 6.707 | 3.230 | 1.00 | 0.00 C | |
| ATOM | 194 | C | GLY A | 17137.602 | 6.015 | 3.375 | 1.00 | 0.00 C | |
| ATOM | 195 | O | GLY A | 17138.004 | 5.653 | 4.481 | 1.00 | 0.00 O | |
| ATOM | 196 | Н | GLY A | 17135.690 | 5.574 | 1.536 | 1.00 | 0.00 H | |
| ATOM | 197 | IHA | GLY A | 17136.421 | 7.695 | 2.823 | 1.00 | 0.00 H | |
| ATOM | 198 2 | 2HA | GLY A | 17135.809 | 6.802 | 4.206 | 1.00 | 0.00 H | |
| ATOM | 199 | N | LEU A | 18138.294 | 5.830 | 2.256 | 1.00 | 0.00 N | |
| ATOM | 200 | CA | LEU A | 18139.598 | 5.176 | 2.264 | 1.00 | 0.00 C | |
| ATOM | 201 | C | LEU A | 18140.706 | 6.174 | 2.579 | 1.00 | 0.00 C | |
| ATOM | 202 | O | LEU A | 18141.119 | 6.952 | 1.718 | 1.00 | 0.00 O | |
| ATOM | 203 | СВ | LEU A | 18139.865 | 4.509 | 0.913 | 1.00 | 0.00 C | |
| ATOM | 204 | CG | LEU A | 18138.793 | 3.519 | 0.456 | 1.00 | 0.00 C | |
| ATOM | 205 | CD1 | LEU A | 18138.995 | 3.149 | -1.004 | 1.00 | 0.00 C | |
| ATOM | 206 | CD2 | LEU A | 18138.812 | 2.274 | 1.330 | 1.00 | 0.00 C | |
| ATOM | 207 | Н | LEU A | 18137.921 | 6.141 | 1.406 | 1.00 | 0.00 H | |
| ATOM | 208 | НА | LEU A | 18139.583 | 4.418 | 3.032 | 1.00 | 0.00 H | |
| ATOM | 209 1 | lНВ | LEU A | 18139.953 | 5.284 | 0.165 | 1.00 | 0.00 H | |
| ATOM | 210 2 | 2HB | LEU A | 18140.806 | 3.983 | 0.975 | 1.00 | 0.00 H | |
| ATOM | 211 | HG | LEU A | 18137.821 | 3.981 | 0.552 | 1.00 | 0.00 H | |
| ATOM | 212 | HD1 | LEU A | 18139.946 | 2.651 | -1.122 | 1.00 | 0.00 H | |
| ATOM | 213 2 | 2HD1 | LEU A | 18138.982 | 4.045 | -1.608 | 1.00 | 0.00 H | |
| ATOM | 214 3 | BHD1 | LEU A | 18138.202 | 2.489 | -1.322 | 1.00 | 0.00 H | |
| ATOM | 215 | HD2 | LEU A | 18139.397 | 1.505 | 0.849 | 1.00 | 0.00 H | |
| ATOM | 216 2 | 2HD2 | LEU A | 18137.802 | 1.920 | 1.475 | 1.00 | 0.00 H | |

| ATOM | 217 | 3HD2 | LEU A | 18139.250 | 2.513 | 2.288 | 1.00 | 0.00 H |
|--------|-----|------|-------|-----------|-------|-------|------|--------|
| ATOM | 218 | N | GLU A | 19141.185 | 6.148 | 3.819 | 1.00 | 0.00 N |
| ATOM | 219 | CA | GLU A | 19142.246 | 7.051 | 4.248 | 1.00 | 0.00 C |
| ATOM . | 220 | C | GLU A | 19143.202 | 6.348 | 5.207 | 1.00 | 0.00 C |
| ATOM | 221 | O | GLU A | 19143.061 | 5.156 | 5.479 | 1.00 | 0.00 O |
| ATOM | 222 | CB | GLU A | 19141.650 | 8.289 | 4.919 | 1.00 | 0.00 C |
| ATOM | 223 | CG | GLU A | 19140.820 | 7.972 | 6.152 | 1.00 | 0.00 C |
| ATOM | 224 | CD | GLU A | 19141.049 | 8.961 | 7.279 | 1.00 | 0.00 C |
| ATOM | 225 | OE1 | GLU A | 19142.219 | 9.330 | 7.517 | 1.00 | 0.00 O |
| ATOM | 226 | OE2 | GLU A | 19140.058 | 9.368 | 7.922 | 1.00 | 0.00 O |
| ATOM | 227 | Н | GLU A | 19140.816 | 5.504 | 4.460 | 1.00 | 0.00 H |
| ATOM | 228 | НА | GLU A | 19142.796 | 7.357 | 3.371 | 1.00 | 0.00 H |
| ATOM | 229 | 1HB | GLU A | 19142.455 | 8.948 | 5.212 | 1.00 | 0.00 H |
| ATOM | 230 | 2HB | GLU A | 19141.018 | 8.800 | 4.209 | 1.00 | 0.00 H |
| ATOM | 231 | 1HG | GLU A | 19139.776 | 7.993 | 5.883 | 1.00 | 0.00 H |
| ATOM | 232 | 2HG | GLU A | 19141.081 | 6.984 | 6.502 | 1.00 | 0.00 H |
| ATOM | 233 | N | VAL A | 20144.175 | 7.096 | 5.717 | 1.00 | 0.00 N |
| ATOM | 234 | CA | VALA | 20145.156 | 6.545 | 6.647 | 1.00 | 0.00 C |
| ATOM | 235 | C | VAL A | 20144.476 | 5.973 | 7.886 | 1.00 | 0.00 C |
| ATOM | 236 | О | VAL A | 20143.563 | 6.582 | 8.443 | 1.00 | 0.00 O |
| ATOM | 237 | CB | VAL A | 20146.178 | 7.612 | 7.081 | 1.00 | 0.00 C |
| ATOM | 238 | CG1 | VAL A | 20147.289 | 6.984 | 7.908 | 1.00 | 0.00 C |
| ATOM | 239 | CG2 | VAL A | 20146.748 | 8.330 | 5.868 | 1.00 | 0.00 C |
| ATOM | 240 | Н | VAL A | 20144.237 | 8.041 | 5.462 | 1.00 | 0.00 H |
| ATOM | 241 | НА | VAL A | 20145.687 | 5.753 | 6.139 | 1.00 | 0.00 H |
| ATOM | 242 | HB | VAL A | 20145.670 | 8.340 | 7.697 | 1.00 | 0.00 H |
| ATOM | 243 | 1HG1 | VAL A | 20146.955 | 6.867 | 8.929 | 1.00 | 0.00 H |

| ATOM | 244 2 | 2HG1 | VALA | 20148.160 | 7.622 | 7.885 | 1.00 | 0.00 H |
|------|-------|------|-------|-----------|--------|--------|------|--------|
| ATOM | 245 | 3HG1 | VAL A | 20147.539 | 6.017 | 7.499 | 1.00 | 0.00 H |
| ATOM | 246 | 1HG2 | VAL A | 20147.025 | 7.605 | 5.117 | 1.00 | 0.00 H |
| ATOM | 247 | 2HG2 | VAL A | 20147.620 | 8.896 | 6.161 | 1.00 | 0.00 H |
| ATOM | 248 | 3HG2 | VALA | 20146.004 | 9.001 | 5.463 | 1.00 | 0.00 H |
| ATOM | 249 | N | GLY A | 21144.928 | 4.797 | 8.312 | 1.00 | 0.00 N |
| ATOM | 250 | CA | GLY A | 21144.352 | 4.163 | 9.482 | 1.00 | 0.00 C |
| ATOM | 251 | C | GLY A | 21143.278 | 3.154 | 9.125 | 1.00 | 0.00 C |
| ATOM | 252 | O | GLY A | 21143.175 | 2.098 | 9.750 | 1.00 | 0.00 O |
| ATOM | 253 | Н | GLY A | 21145.658 | 4.358 | 7.827 | 1.00 | 0.00 H |
| ATOM | 254 | l HA | GLY A | 21145.137 | 3.658 | 10.028 | 1.00 | 0.00 H |
| ATOM | 255 2 | 2HA | GLY A | 21143.920 | 4.923 | 10.116 | 1.00 | 0.00 H |
| ATOM | 256 | N | SER A | 22142.474 | 3.480 | 8.118 | 1.00 | 0.00 N |
| ATOM | 257 | CA | SER A | 22141.402 | 2.595 | 7.678 | 1.00 | 0.00 C |
| ATOM | 258 | C | SER A | 22141.949 | 1.470 | 6.805 | 1.00 | 0.00 C |
| ATOM | 259 | O | SER A | 22142.939 | 1.645 | 6.095 | 1.00 | 0.00 O |
| ATOM | 260 | CB | SER A | 22140.344 | 3.385 | 6.907 | 1.00 | 0.00 C |
| ATOM | 261 | OG | SER A | 22140.269 | 4.723 | 7.368 | 1.00 | 0.00 O |
| ATOM | 262 | Н | SER A | 22142.606 | 4.335 | 7.659 | 1.00 | 0.00 H |
| ATOM | 263 | НА | SER A | 22140.947 | 2.164 | 8.556 | 1.00 | 0.00 H |
| ATOM | 264 | 1HB | SER A | 22140.598 | 3.395 | 5.857 | 1.00 | 0.00 H |
| ATOM | 265 2 | 2HB | SER A | 22139.380 | 2.916 | 7.039 | 1.00 | 0.00 H |
| ATOM | 266 | HG | SER A | 22140.281 | 4.731 | 8.329 | 1.00 | 0.00 H |
| ATOM | 267 | N | LEU A | 23141.298 | 0.312 | 6.864 | 1.00 | 0.00 N |
| ATOM | 268 | CA | LEU A | 23141.719 | -0.842 | 6.079 | 1.00 | 0.00 C |
| ATOM | 269 | C | LEU A | 23141.156 | -0.772 | 4.664 | 1.00 | 0.00 C |
| ATOM | 270 | О | LEU A | 23140.073 | -0.229 | 4.441 | 1.00 | 0.00 O |

ATOM CB LEUA 23141.267 -2.138 6.756 1.00 0.00 C 271 CG LEUA 23141.762 -2.325 8.192 1.00 0.00 C **ATOM** 272 **ATOM** CD1 LEU A 23140.763 -3.143 8.997 1.00 0.00 C 273 CD2 LEU A 23143.129 -2.990 8.201 1.00 0.00 C **ATOM** 274 **ATOM** 275 Η LEUA 23140.515 0.233 7.449 1.00 0.00 H 276 HA LEUA 23142.797 -0.831 6.026 1.00 0.00 H **ATOM** 277 1HB LEUA 23140.186 -2.158 6.763 1.00 0.00 H **ATOM ATOM** 278 2HB LEU A 23141.622 -2.970 6.167 1.00 0.00 H 279 HG LEUA 23141.855 -1.357 8.662 1.00 0.00 H **ATOM** 280 1HD1 LEU A 23140.721 -2.76510.008 1.00 0.00 H **ATOM ATOM** 281 2HD1 LEU A 23141.074 -4.177 9.012 1.00 0.00 H282 3HD1 LEU A 23139.786 -3.066 8.544 1.00 0.00 H**ATOM** 283 1HD2 LEU A 23143.718 -2.591 9.013 1.00 0.00 H **ATOM** 284 2HD2 LEU A 23143.630 -2.796 7.264 1.00 0.00 H**ATOM** 285 3HD2 LEU A 23143.010 -4.056 8.332 1.00 0.00 H **ATOM ATOM** 286 N ALAA 24141.896 -1.326 3.709 1.00 0.00 N **ATOM** 287 CA ALAA 24141.472 -1.326 2.314 1.00 0.00 C ALAA 24142.116 -2.474 1.545 1.00 0.00 C **ATOM** 288 C **ATOM** 289 O ALAA 24143.252 -2.858 1.820 1.00 0.00 O ALA A 24141.806 0.005 1.660 1.00 0.00 C **ATOM** 290 CB 24142.750 -1.744 3.949 1.00 0.00 H **ATOM** 291 Η **ALAA** 292 HA ALAA 24140.398 -1.451 2.294 1.00 0.00 H**ATOM** 293 1HB ALAA 24142.746 -0.079 1.134 1.00 0.00 H **ATOM** 294 2HB ALAA 24141.884 0.770 2.419 1.00 0.00 H**ATOM** 0.962 1.00 0.00 H ALAA 24141.026 0.270 **ATOM** 295 3HB 0.578 1.00 0.00 N GLU A 25141.383 -3.016 **ATOM** 296 N -0.233 1.00 0.00 C **ATOM** 297 CA GLUA 25141.883 -4.121

| ATOM | 298 | C | GLU A | 25142.149 | -3.669 | -1.665 | 1.00 | 0.00 C |
|------|-----|------|-------|-----------|--------|--------|------|--------|
| ATOM | 299 | О | GLU A | 25141.544 | -2.711 | -2.146 | 1.00 | 0.00 O |
| ATOM | 300 | CB | GLU A | 25140.883 | -5.278 | -0.229 | 1.00 | 0.00 C |
| ATOM | 301 | CG | GLU A | 25141.402 | -6.533 | -0.912 | 1.00 | 0.00 C |
| ATOM | 302 | CD | GLU A | 25140.359 | -7.631 | -0.983 | 1.00 | 0.00 C |
| ATOM | 303 | OE1 | GLU A | 25140.483 | -8.511 | -1.860 | 1.00 | 0.00 O |
| ATOM | 304 | OE2 | GLU A | 25139.420 | -7.612 | -0.159 | 1.00 | 0.00 O |
| ATOM | 305 | H | GLU A | 25140.484 | -2.666 | 0.406 | 1.00 | 0.00 H |
| ATOM | 306 | HA | GLU A | 25142.812 | -4.458 | 0.203 | 1.00 | 0.00 H |
| ATOM | 307 | 1HB | GLU A | 25140.640 | -5.526 | 0.794 | 1.00 | 0.00 H |
| ATOM | 308 | 2HB | GLU A | 25139.984 | -4.963 | -0.738 | 1.00 | 0.00 H |
| ATOM | 309 | 1HG | GLU A | 25141.704 | -6.281 | -1.917 | 1.00 | 0.00 H |
| ATOM | 310 | 2HG | GLU A | 25142.255 | -6.900 | -0.362 | 1.00 | 0.00 H |
| ATOM | 311 | N | VAL A | 26143.058 | -4.363 | -2.340 | 1.00 | 0.00 N |
| ATOM | 312 | CA | VAL A | 26143.405 | -4.034 | -3.718 | 1.00 | 0.00 C |
| ATOM | 313 | C | VAL A | 26143.016 | -5.163 | -4.667 | 1.00 | 0.00 C |
| ATOM | 314 | O | VAL A | 26142.958 | -6.327 | -4.272 | 1.00 | 0.00 O |
| ATOM | 315 | CB | VAL A | 26144.911 | -3.750 | -3.867 | 1.00 | 0.00 C |
| ATOM | 316 | CG1 | VAL A | 26145.220 | -3.217 | -5.257 | 1.00 | 0.00 C |
| ATOM | 317 | CG2 | VAL A | 26145.378 | -2.775 | -2.798 | 1.00 | 0.00 C |
| ATOM | 318 | Н | VAL A | 26143.507 | -5.116 | -1.903 | 1.00 | 0.00 H |
| ATOM | 319 | НА | VAL A | 26142.862 | -3.141 | -3.995 | 1.00 | 0.00 H |
| ATOM | 320 | НВ | VAL A | 26145.446 | -4.679 | -3.735 | 1.00 | 0.00 H |
| ATOM | 321 | 1HG1 | VALA | 26146.167 | -2.698 | -5.241 | 1.00 | 0.00 H |
| ATOM | 322 | 2HG1 | VAL A | 26144.441 | -2.535 | -5.563 | 1.00 | 0.00 H |
| ATOM | 323 | 3HG1 | VALA | 26145.272 | -4.039 | -5.955 | 1.00 | 0.00 H |
| ATOM | 324 | 1HG2 | VAL A | 26144.985 | -3.076 | -1.838 | 1.00 | 0.00 H |

| ATOM | 325 2 | HG2 | VAL A | 26145.026 | -1.782 | -3.036 | 1.00 | 0.00 H |
|------|-------|-----|-------|-----------|-----------|-----------------|------|--------|
| ATOM | 326 3 | HG2 | VAL A | 26146.458 | -2.773 | -2.759 | 1.00 | 0.00 H |
| ATOM | 327 | N | LYS A | 27142.751 | -4.810 | -5.921 | 1.00 | 0.00 N |
| ATOM | 328 | CA | LYS A | 27142.369 | -5.793 | -6.927 | 1.00 | 0.00 C |
| ATOM | 329 | C | LYS A | 27143.583 | -6.248 | -7.731 , | 1.00 | 0.00 C |
| ATOM | 330 | O | LYS A | 27144.100 | -5.507 | -8.567 | 1.00 | 0.00 O |
| ATOM | 331 | CB | LYS A | 27141.311 | -5.209 | -7.865 | 1.00 | 0.00 C |
| ATOM | 332 | CG | LYS A | 27140.596 | -6.257 | -8.703 | 1.00 | 0.00 C |
| ATOM | 333 | CD | LYS A | 27139.384 | -5.672 | -9.410 | 1.00 | 0.00 C |
| ATOM | 334 | CE | LYS A | 27139.017 | -6.478 - | 10.646 | 1.00 | 0.00 C |
| ATOM | 335 | NZ | LYS A | 27137.542 | -6.568 - | 10.832 | 1.00 | 0.00 N |
| ATOM | 336 | Н | LYS A | 27142.815 | -3.865 | -6.176 | 1.00 | 0.00 H |
| ATOM | 337 | НА | LYS A | 27141.951 | -6.647 | -6.414 | 1.00 | 0.00 H |
| ATOM | 338 1 | НВ | LYS A | 27140.573 | -4.686 | -7.276 | 1.00 | 0.00 H |
| ATOM | 339 2 | 2HB | LYS A | 27141.787 | -4.509 | -8.535 | 1.00 | 0.00 H |
| ATOM | 340 1 | HG | LYS A | 27141.280 | -6.641 | -9.443 | 1.00 | 0.00 H |
| ATOM | 341 2 | 2HG | LYS A | 27140.271 | -7.060 | -8.057 | 1.00 | 0.00 H |
| ATOM | 342 1 | HD | LYS A | 27138.545 | -5.673 | -8.729 | 1.00 | 0.00 H |
| ATOM | 343 2 | 2HD | LYS A | 27139.607 | -4.657 | -9.707 | 1.00 | 0.00 H |
| ATOM | 344 1 | HE | LYS A | 27139.452 | -6.003 -1 | 11.512 | 1.00 | 0.00 H |
| ATOM | 345 2 | 2HE | LYS A | 27139.419 | -7.475 -1 | 10.542 | 1.00 | 0.00 H |
| ATOM | 346 1 | HZ | LYS A | 27137.058 | -6.447 | -9.919 | 1.00 | 0.00 H |
| ATOM | 347 2 | 2HZ | LYS A | 27137.287 | -7.496 -1 | 11.226 | 1.00 | 0.00 H |
| ATOM | 348 3 | BHZ | LYS A | 27137.218 | -5.825 -1 | 11.485 | 1.00 | 0.00 H |
| ATOM | .349 | N | GLU A | 28144.031 | -7.473 | -7.475 | 1.00 | 0.00 N |
| ATOM | 350 | CA | GLU A | 28145.184 | -8.026 | -8.174 | 1.00 | 0.00 C |
| ATOM | 351 | C | GLU A | 28145.135 | -9.551 | -8.180 | 1.00 | 0.00 C |

GLU A 28144.125 -10.152 -7.814 0.00 O 0 1.00 **ATOM** 352 GLUA 28146.483 -7.545 -7.523 1.00 0.00 C **ATOM** CB 353 1.00 **ATOM** 354 CG GLU A 28147.503 -7.017 -8.517 0.00 C CD GLUA 28148.752 -7.873 -8.585 1.00 0.00 C **ATOM** 355 356 OE1 GLUA 28149.528 -7.872 -7.606 1.00 0.00 O **ATOM ATOM** 357 OE2 GLU A 28148.955 -8.548 -9.617 1.00 0.00 O GLUA 28143.576 -8.016 -6.798 1.00 0.00 H **ATOM** Η 358 GLUA 28145.152 -7.674 -9.194 1.00 0.00 H **ATOM** HA 359 -6.824 1.00 360 1HB GLUA 28146.249 -6.755 0.00 H **ATOM** -6.983 1.00 0.00 H GLUA 28146.929 -8.368 **ATOM** 361 2HB **ATOM** 362 1HG GLU A 28147.052 -6.989 -9.497 1.00 0.00 H -8.224 1.00 0.00 H**ATOM** 363 2HG GLU A 28147.786 -6.016 -8.599 1.00 0.00 N ASN A 29146.234 -10.172 **ATOM** 364 N 29146.317 -11.626 -8.650 1.00 0.00 C **ATOM** 365 CA ASN A 29146.467 -12.213 -7.249 1.00 0.00 C C ASN A **ATOM** 366 **ATOM** 367 O ASN A 29145.645 -13.020 -6.814 1.00 0.00 O 29147.493 -12.059 0.00 C CBASN A -9.529 1.00 **ATOM** 368 29147.063 -12.398 -10.943 1.00 0.00 C **ATOM** 369 CG ASN A OD1 ASN A 29146.874 -13.566 -11.284 1.00 0.00 O **ATOM** 370 29146.907 -11.375 -11.776 1.00 0.00 N ND2 ASN A **ATOM** 371 29147.008 -9.638 -8.876 1.00 0.00 H **ATOM** 372 Н ASN A HA ASN A 29145.400 -11.995 -9.085 1.00 0.00 H **ATOM** 373 ASN A 29148.214 -11.257 -9.576 1.00 0.00 H **ATOM** 374 1HB 375 2HB ASN A 29147.958 -12.932 -9.095 1.00 0.00 H**ATOM** 0.00 H 376 1HD2 ASN A 29147.076 -10.472 -11.435 1.00 **ATOM** 0.00 H377 2HD2 ASN A 29146.629 -11.566 -12.696 1.00 **ATOM ATOM** 378 N PRO A 30147.526 -11.816 -6.522

| ATOM | 379 | CA | PRO A | 30147.782 -12.306 | -5.166 | 1.00 | 0.00 C |
|------|-------|-----|-------|-------------------|--------|------|--------|
| ATOM | 380 | C | PRO A | 30146.884 -11.635 | -4.126 | 1.00 | 0.00 C |
| ATOM | 381 | O | PRO A | 30147.049 -10.453 | -3.828 | 1.00 | 0.00 O |
| ATOM | 382 | СВ | PRO A | 30149.243 -11.926 | -4.932 | 1.00 | 0.00 C |
| ATOM | 383 | CG | PRO A | 30149.448 -10.704 | -5.760 | 1.00 | 0.00 C |
| ATOM | 384 | CD | PRO A | 30148.557 -10.856 | -6.965 | 1.00 | 0.00 C |
| ATOM | 385 | НА | PRO A | 30147.671 -13.378 | -5.105 | 1.00 | 0.00 H |
| ATOM | 386 1 | НВ | PRO A | 30149.403 -11.727 | -3.883 | 1.00 | 0.00 H |
| ATOM | 387 2 | НВ | PRO A | 30149.884 -12.733 | -5.255 | 1.00 | 0.00 H |
| ATOM | 388 1 | HG | PRO A | 30149.166 -9.829 | -5.194 | 1.00 | 0.00 H |
| ATOM | 389 2 | HG | PRO A | 30150.482 -10.638 | -6.064 | 1.00 | 0.00 H |
| ATOM | 390 1 | HD | PRO A | 30148.113 -9.908 | -7.225 | 1.00 | 0.00 H |
| ATOM | 391 2 | HD | PRO A | 30149.117 -11.252 | -7.799 | 1.00 | 0.00 H |
| ATOM | 392 | N | PRO A | 31145.919 -12.382 | -3.559 | 1.00 | 0.00 N |
| ATOM | 393 | CA | PRO A | 31145.001 -11.844 | -2.550 | 1.00 | 0.00 C |
| ATOM | 394 | C | PRO A | 31145.700 -11.555 | -1.226 | 1.00 | 0.00 C |
| ATOM | 395 | О | PRO A | 31146.226 -12.461 | -0.579 | 1.00 | 0.00 O |
| ATOM | 396 | CB | PRO A | 31143.968 -12.960 | -2.376 | 1.00 | 0.00 C |
| ATOM | 397 | CG | PRO A | 31144.686 -14.204 | -2.768 | 1.00 | 0.00 C |
| ATOM | 398 | CĎ | PRO A | 31145.648 -13.802 | -3.851 | 1.00 | 0.00 C |
| ATOM | 399 | HA | PRO A | 31144.511 -10.946 | -2.899 | 1.00 | 0.00 H |
| ATOM | 400 1 | HB | PRO A | 31143.644 -12.996 | -1.346 | 1.00 | 0.00 H |
| ATOM | 401 2 | 2HB | PRO A | 31143.121 -12.775 | -3.019 | 1.00 | 0.00 H |
| ATOM | 402 1 | HG | PRO A | 31145.224 -14.600 | -1.918 | 1.00 | 0.00 H |
| ATOM | 403 2 | 2HG | PRO A | 31143.982 -14.932 | -3.142 | 1.00 | 0.00 H |
| ATOM | 404 1 | HD | PRO A | 31146.553 -14.388 | -3.790 | 1.00 | 0.00 H |
| ATOM | 405 2 | 2HD | PRO A | 31145.189 -13.914 | -4.822 | 1.00 | 0.00 H |

| ATOM | 406 | N | PHE A | 32145.703 - | -10.287 | -0.828 | 1.00 | 0.00 N |
|------|-------|-----|-------|-------------|---------|--------|------|--------|
| ATOM | 407 | CA | PHE A | 32146.338 | -9.878 | 0.420 | 1.00 | 0.00 C |
| ATOM | 408 | C | PHE A | 32145.479 | -8.858 | 1.160 | 1.00 | 0.00 C |
| ATOM | 409 | Ο | PHE A | 32144.591 | -8.238 | 0.574 | 1.00 | 0.00 O |
| ATOM | 410 | СВ | PHE A | 32147.723 | -9.291 | 0.142 | 1.00 | 0.00 C |
| ATOM | 411 | CG | PHE A | 32147.736 | -8.287 | -0.975 | 1.00 | 0.00 C |
| ATOM | 412 | CD1 | PHE A | 32148.424 | -8.547 | -2.150 | 1.00 | 0.00°C |
| ATOM | 413 | CD2 | PHE A | 32147.060 | -7.083 | -0.851 | 1.00 | 0.00 C |
| ATOM | 414 | CE1 | PHE A | 32148.438 | -7.626 | -3.180 | 1.00 | 0.00 C |
| ATOM | 415 | CE2 | PHE A | 32147.070 | -6.158 | -1.878 | 1.00 | 0.00 C |
| ATOM | 416 | CZ | PHE A | 32147.760 | -6.429 | -3.044 | 1.00 | 0.00 C |
| ATOM | 417 | Н | PHE A | 32145.267 | -9.610 | -1.386 | 1.00 | 0.00 H |
| ATOM | 418 | HA | PHE A | 32146.447 | -10.756 | 1.038 | 1.00 | 0.00 H |
| ATOM | 419 1 | lНВ | PHE A | 32148.083 | -8.799 | 1.033 | 1.00 | 0.00 H |
| ATOM | 420 2 | 2HB | PHE A | 32148.399 | -10.090 | -0.120 | 1.00 | 0.00 H |
| ATOM | 421 | HD1 | PHE A | 32148.955 | -9.482 | -2.257 | 1.00 | 0.00 H |
| ATOM | 422 | HD2 | PHE A | 32146.521 | -6.871 | 0.060 | 1.00 | 0.00 H |
| ATOM | 423 | HE1 | PHE A | 32148.978 | -7.839 | -4.090 | 1.00 | 0.00 H |
| ATOM | 424 | HE2 | PHE A | 32146.540 | -5.224 | -1.769 | 1.00 | 0.00 H |
| ATOM | 425 | HZ | PHE A | 32147.770 | -5.708 | -3.847 | 1.00 | 0.00 H |
| ATOM | 426 | N | TYR A | 33145.750 | -8.690 | 2.450 | 1.00 | 0.00 N |
| ATOM | 427 | CA | TYR A | 33145.001 | -7.746 | 3.272 | 1.00 | 0.00 C |
| ATOM | 428 | C | TYR A | 33145.945 | -6.812 | 4.022 | 1.00 | 0.00 C |
| ATOM | 429 | О | TYR A | 33146.943 | -7.251 | 4.594 | 1.00 | 0.00 O |
| ATOM | 430 | CB | TYR A | 33144.109 | -8.494 | 4.264 | 1.00 | 0.00 C |
| ATOM | 431 | CG | TYR A | 33142.774 | -8.908 | 3.687 | 1.00 | 0.00 C |
| ATOM | 432 | CD1 | TYR A | 33142.316 | -10.213 | 3.813 | 1.00 | 0.00 C |

| ATOM | 433 | CD2 | TYR A | 33141.973 | -7.993 | 3.014 | 1.00 | 0.00 C |
|------|-----|-----|-------|-------------|---------|-------|------|--------|
| ATOM | 434 | CE1 | TYR A | 33141.097 - | 10.594 | 3.287 | 1.00 | 0.00 C |
| ATOM | 435 | CE2 | TYR A | 33140.752 | -8.368 | 2.486 | 1.00 | 0.00 C |
| ATOM | 436 | CZ | TYR A | 33140.319 | -9.668 | 2.625 | 1.00 | 0.00 C |
| ATOM | 437 | ОН | TYR A | 33139.104 | -10.045 | 2.099 | 1.00 | 0.00 O |
| ATOM | 438 | Н | TYR A | 33146.469 | -9.214 | 2.860 | 1.00 | 0.00 H |
| ATOM | 439 | НА | TYR A | 33144.379 | -7.156 | 2.615 | 1.00 | 0.00 H |
| ATOM | 440 | 1HB | TYR A | 33144.620 | -9.387 | 4.592 | 1.00 | 0.00 H |
| ATOM | 441 | 2HB | TYR A | 33143.921 | -7.859 | 5.117 | 1.00 | 0.00 H |
| ATOM | 442 | HD1 | TYR A | 33142.927 | -10.935 | 4.333 | 1.00 | 0.00 H |
| ATOM | 443 | HD2 | TYR A | 33142.316 | -6.975 | 2.907 | 1.00 | 0.00 H |
| ATOM | 444 | HE1 | TYR A | 33140.757 - | 11.614 | 3.396 | 1.00 | 0.00 H |
| ATOM | 445 | HE2 | TYR A | 33140.144 | -7.642 | 1.967 | 1.00 | 0.00 H |
| ATOM | 446 | НН | TYR A | 33138.462 | -10.131 | 2.807 | 1.00 | 0.00 H |
| ATOM | 447 | N | GLY A | 34145.623 | -5.522 | 4.016 | 1.00 | 0.00 N |
| ATOM | 448 | CA | GLY A | 34146.453 | -4.548 | 4.700 | 1.00 | 0.00 C |
| ATOM | 449 | C | GLY A | 34145.682 | -3.302 | 5.091 | 1.00 | 0.00 C |
| ATOM | 450 | O | GLY A | 34144.454 | -3.272 | 5.009 | 1.00 | 0.00°O |
| ATOM | 451 | Н | GLY A | 34144.817 | -5.230 | 3.543 | 1.00 | 0.00 H |
| ATOM | 452 | 1HA | GLY A | 34146.861 | -5.001 | 5.591 | 1.00 | 0.00 H |
| ATOM | 453 | 2HA | GLY A | 34147.267 | -4.264 | 4.049 | 1.00 | 0.00 H |
| ATOM | 454 | N | VAL A | 35146.405 | -2.272 | 5.520 | 1.00 | 0.00 N |
| ATOM | 455 | CA | VAL A | 35145.783 | -1.018 | 5.927 | 1.00 | 0.00 C |
| ATOM | 456 | C | VAL A | 35146.505 | 0.177 | 5.313 | 1.00 | 0.00 C |
| ATOM | 457 | О | VAL A | 35147.721 | 0.150 | 5.125 | 1.00 | 0.00 O |
| ATOM | 458 | СВ | VAL A | 35145.769 | -0.870 | 7.462 | 1.00 | 0.00 C |
| ATOM | 459 | CG1 | VALA | 35147.188 | -0.848 | 8.012 | 1.00 | 0.00 C |

CG2 VAL A 35145.010 7.873 1.00 0.00 C **ATOM** 460 0.383 1.00 0.00 H 35147.380 -2.359 5.565 **ATOM** 461 Η VALA HA VAL A 35144.760 -1.026 5.579 1.00 0.00 H **ATOM** 462 7.880 1.00 0.00 H **ATOM** HB VAL A 35145.261 -1.726 463 -1.287 7.291 1.00 0.00 H 464 1HG1 VAL A 35147.862 **ATOM ATOM** 465 2HG1 VALA 35147.226 -1.413 8.931 1.00 0.00 H 8.204 1.00 0.00 H466 3HG1 VAL A 35147.483 0.173 **ATOM** 7.654 1.00 0.00 H467 1HG2 VAL A 35143.960 0.255 **ATOM** 1.00 7.324 0.00 H**ATOM** 468 2HG2 VAL A 35145.392 1.231 1.00 0.00 H0.551 8.931 469 3HG2 VAL A 35145.140 **ATOM** 470 N ILE A 36145.747 1.224 5.003 1.00 0.00 N **ATOM** 1.00 0.00 C CA ILE A 36146.316 2.429 4.411 **ATOM** 471 1.00 0.00 C 36147.242 3.136 5.395 \mathbf{C} ILE A **ATOM** 472 1.00 0.00 O 473 O ILE A 36146.961 3.200 6.592 **ATOM** 3.960 1.00 0.00 C CB ILE A 36145.216 3.410 **ATOM** 474 CG1 ILE A 36144.192 2.693 3.078 1.00 0.00 C **ATOM** 475 CG2 ILE A 36145.828 4.590 3.218 1.00 0.00 C **ATOM** 476 2.627 1.00 0.00 C **ATOM** 477 CD1 ILE A 36143.055 3.584 Η ILE A 36144.783 1.186 5.177 1.00 0.00 H **ATOM** 478 3.542 1.00 0.00 H ILE A 36146.887 2.136 **ATOM** 479 HA ILE A 3.789 4.841 1.00 0.00 H HB 36144.720 **ATOM** 480 481 1HG1 ILE A 36144.686 2.316 2.196 1.00 0.00 H **ATOM** 0.00 H 482 2HG1 ILE A 36143.767 1.866 3.629 1.00 **ATOM** 483 1HG2 ILE A 36146.782 4.299 2.805 1.00 0.00 H**ATOM** 484 2HG2 ILE A 36145.968 1.00 0.00 H5.413 3.903 **ATOM** 1.00 0.00 H36145.168 4.894 2.420 485 3HG2 ILE A **ATOM** 1.00 0.00 H**ATOM** 486 1HD1 ILE A 36143.454 4.434 2.094